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THE SCATTERING OPERATOR IN QUANTUM MECHANICS

PART II: THE SCATTERING OPERATOR FORMALISM AND OTHER FORMALISMS

by

H. E. MOSES

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Part II: The Scattering Operator Formalism and Other Formalisms

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H. E. Moses

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Morris Kline
Project Director

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ABSTRACT

With the aid of a scattering operator it is often possible to formulate and solve scattering problems more clearly and concisely than by conventional procedures. We define the scattering operator by means of the time-dependent Schroedinger equation, give some of its properties, and indicate the relationship between the scattering operator formalism and more conventional formalisms.

Note. This investigation has been divided into two parts. In Part I the scattering operator was defined and some of its properties discussed. In Part II we discuss the relationship of the scattering operator formalism to other formalisms. The numbering of the pages, sections, appendices, and bibliography continues from Part I. Part I appeared in this series of reports as Research Report CX-12.

12. Variational Principles for the Scattering Operator.

In scattering problems we are interested in obtaining the quantity $T_-(E,\alpha|E,\alpha')$, that is, "the amplitude of the scattered wave." If we knew $u_-(F,\alpha|F,\beta)$ exactly, it would be possible to find $T_-(E,\alpha|E,\alpha')$ exactly by means of the definition of T_- (eq. 6.28). The calculation of T_- by such a procedure is thus equivalent to the solving of the integral equation for u_-. One would like to have simpler methods of obtaining T_-, even if it meant obtaining an approximate instead of an exact expression. The most obvious method of obtaining an approximate result is to use a function which approximates u_- directly in the defining equation for T_-. However, it is possible to get more accurate results for $T_-(E,\alpha|E,\alpha')$ by substituting such an approximate function, which we shall call a trial function, into variational expressions which are not sensitive to this function.

There are two variational principles in common use: the Schwinger variational principle, and the Kohn-Hulthen variational principle. Kato (ref. 14) and Kohn (ref. 15) have shown these to be equivalent in the case of the scattering of a single particle. The two variational principles are presumably equivalent in general, though no explicit proof has thus far been given. However, we shall discuss these variational principles as though they were independent. In particular, the Kohn-Hulthen method will be discussed in a more general way than is commonly done.

A. The Schwinger Variational Principle.

Schwinger's variational principle can be set up in a simple form in terms of the H_o representation. We shall, however, first consider the principle abstractly.

Consider the two equations

$$a = Ky \qquad (12.01)$$
$$a' = K'y'$$

where a, a', y, y' are vectors, K is an operator and K' is the Hermitian adjoint of K defined by

$$(a,Kb) = (K'a,b). \qquad (12.02)$$

One can then prove the reciprocity relation

$$(12.03) \qquad (a',y) = (y', a)$$

directly from (12.01) and (12.02). We define λ by

$$(12.04) \qquad \lambda = \frac{1}{(a',y)} = \frac{1}{(y',a)}$$

and the "functional" $\lambda(v',v)$ by

$$(12.05) \qquad \lambda(v',v) = \frac{(v',Kv)}{(a',v)(v',a)} .$$

Hence

$$(12.06) \qquad \lambda(y',y) = \lambda .$$

The functional $\lambda(v',v)$ is stationary for independent variations of v and v' about the values y and y' respectively, and, therefore, the stationary value of $\lambda(v',v)$ is λ. We prove this statement as follows: Let us consider the variation of $\lambda(v',v)$ around $v' = y'$, $v = y$ with respect to the second variable. Denoting the variations with respect to the second variable by $\delta_v(v',v)$ we have,

$$(12.07) \qquad \begin{aligned} \delta_v\lambda(v',v) &= \lambda(y', y+\delta y) - \lambda(y',y) \\ &= \lambda(y', y+\delta y) - \lambda \\ &= \frac{(y',Ky) + (y',K\delta y)}{(y',a)\left[(a',y) + (a',\delta y)\right]} - \lambda . \end{aligned}$$

Expanding the right hand side to the first order in δy, we have

$$\delta_v\lambda(v',v) = \frac{(y',Ky)}{(y',a)(a',y)} + \frac{(y',K\delta y)}{(y',a)(a',y)} - \frac{(y',Ky)(a',\delta y)}{(y',a)(a',y)(a',y)} - \lambda .$$

The first term on the right equals λ. Hence using (12.01),

$$(12.08) \qquad \delta_v\lambda(v',v) = \frac{(K'y',\delta y)}{(y',a)(a',y)} - \frac{(y',Ky)(a',\delta y)}{(y',a)(a',y)(a',y)} = 0.$$

In a similar way it can be shown that to the first order in $\delta y'$

$$(12.09) \qquad \delta_{v'}\lambda(v',v) = \lambda(y'+\delta y',y)-\lambda(y',y) = 0.$$

Hence we have proved that $\lambda(v',v)$ is stationary for independent variations about $v = y$, $v' = y'$. The variation in $\lambda(v',v)$ produced by an arbitrary variation (as opposed to an independent variation) about $v' = y'$ and $v = y$ is given by

$$\delta\lambda(v',v) = \lambda(y'+\delta y',y+\delta y)-\lambda(y',y)$$

$$= \delta_{v'}\lambda(v',v)\delta y' + \delta_v\lambda(v',v)\delta y$$

to the first order in $\delta y'$ and δy. Hence from (12.08) and (12.09)

$$(12.10) \qquad \delta\lambda(v',v) = 0.$$

We may conclude that $\lambda(v',v)$ is an insensitive functional of v' and v in the vicinity of $v' = y'$ and $v = y$ and will approximate λ to the second order in the variations δy and $\delta y'$.

In our present problem we shall identify λ with $\frac{1}{T_-(F,\beta'|F,\beta)}$ and thereby obtain a variational method for finding $T_-(F,\beta'|F,\beta)$. (The use of the variables F,β,β' instead of E,α,α' respectively, in T_- is merely for convenience).

We shall now carry out the identification of the quantities appearing in the scattering operator formulation with the quantities appearing in the abstract formulation of Schwinger's variational principle in detail.

The equations for u_- and u_+ may be written, (see (6.27) and (6.28)),

$$(12.11) \qquad V^E(E,\alpha|F,\beta) = \int_{E_a}^{E_b}\int K(E,\alpha|E',\alpha')u_-(E',\alpha'|F,\beta)d\alpha'dE'$$

$$(12.12)\qquad V^E(E,\alpha|F,\beta') = \int_{E_a}^{E_b}\int K'(E,\alpha|E',\alpha')u_+(E',\alpha'|F,\beta')d\alpha' dE'$$

where

$$(12.13)\qquad K(E,\alpha|E',\alpha') = V^E(E,\alpha|E',\alpha') - \varepsilon\int_{E_a}^{E_b}\int V^E(E,\alpha|E'',\alpha'')\gamma_-(F-E'')$$

$$\cdot\, V^E(E'',\alpha''|E',\alpha')d\alpha'' dE''$$

$$(12.14)\qquad K'(E,\alpha|E',\alpha') = V^E(E,\alpha|E',\alpha') - \varepsilon\int_{E_a}^{E_b}\int V^E(E,\alpha|E'',\alpha'')\gamma_+(F-E'')$$

$$\cdot\, V^E(E'',\alpha''|E',\alpha')d\alpha'' dE'' .$$

It is clear that since V is Hermitian

$$(12.15)\qquad \overline{K}(E,\alpha|E',\alpha') = K'(E',\alpha'|E,\alpha) .$$

Hence $K(E,\alpha|E',\alpha')$ and $K'(E,\alpha|E',\alpha')$ are matrices of Hermitian adjoint operators.

We regard the variables F,β,β' as being fixed parameters and identify the first of equations (12.01) with (12.11) as follows: the vector a of equation (12.01) with $V^E(E,\alpha|F,\beta)$, the operator K with the operator whose matrix is $K(E,\alpha|E',\alpha')$, and the vector y with $u_-(E,\alpha|F,\beta)$. In a similar way we can identify a', K', y' of (12.01) with appropriate entities appearing in(12.12).

It is seen that (a', y) is given by

$$(12.16)\qquad \int_{E_a}^{E_b}\int \overline{V}^E(E,\alpha|F,\beta')u_-(E,\alpha|F,\beta)d\alpha dE = \int_{E_a}^{E_b}\int V^E(F,\beta'|E,\alpha)u_-(E,\alpha|F,\beta)d\alpha dE$$

$$= T_-(F,\beta'|F,\beta) = \lambda$$

The reciprocity relation (12.03) is the important reciprocity relation discussed earlier, namely,

$$T_-(F,\beta'|F,\beta) = \overline{T}_+(F,\beta|F,\beta'). \tag{12.17}$$

The identifications which we have made prove (12.17).

The functional whose extremal is λ is written

$$\lambda(v_+,v_-) = \frac{\int_{E_a}^{E_b}\iint_{E_a}^{E_b}\overline{v}_+(E,\alpha|F,\beta')K(E,\alpha|E',\alpha')v_-(E',\alpha'|F,\beta)d\alpha' dE' d\alpha dE}{\left(\int_{E_a}^{E_b}\overline{V}^E(E,\alpha|F,\beta')v_-(E,\alpha|F,\beta)d\alpha dE\right)\left(\int_{E_a}^{E_b}\overline{v}_+(E,\alpha|F,\beta')V^E(E,\alpha|F,\beta)d\alpha dE\right)} \tag{12.18}$$

where $v_+(E,\alpha|F,\beta')$ and $v_-(E,\alpha|F,\beta)$ approximate $u_+(E,\alpha|F,\beta')$ and $u_-(E,\alpha|F,\beta)$, respectively. If, as an approximation, we take the Born approximation as trial functions,

$$v_+(E,\alpha|F,\beta') = \delta(E-F)\delta(\alpha,\beta')$$

$$v_-(E,\alpha|F,\beta) = \delta(E-F)\delta(\alpha,\beta)$$

we obtain

$$\frac{1}{T_-(F,\beta'|F,\beta)} \simeq \frac{K(F,\beta'|F,\beta)}{\overline{V}^E(F,\beta|F,\beta')V^E(F,\beta'|F,\beta)}$$

or

$$T_-(F,\beta'|F,\beta) \simeq \frac{\overline{V}^E(F,\beta|F,\beta')V^E(F,\beta'|F,\beta)}{V^E(F,\beta'|F,\beta) - \epsilon\int_{E_a}^{E_b}\int V^E(F,\beta'|E'',\alpha'')\,\gamma_-(F-E'')\,V^E(E'',\alpha''|F,\beta)\,d\alpha'' dE''}$$

$$\tilde{=} V^E(F,\beta'|F,\beta)+\varepsilon\int_{E_a}^{E_b}\int V^E(F,\beta'|E'',\alpha'')\gamma\ (F-E'')\ V^E(E'',\alpha''|F,\beta)d\alpha''dE''+O(\varepsilon^2).$$

The first two terms of this last expression is the result which would be obtained by using the second Born approximation for u_- in equation (6.28) in which T_- is defined.

B. The Kohn-Hulthen Variational Principle.

The Kohn-Hulthen variational principle is based upon variations of the functional $A(\mathcal{T}_\pm)$ given by

$$A(\mathcal{T}_\pm) = I(\mathcal{T}_\pm) + \varepsilon\mathcal{T}_-(F,\beta'|F,\beta) \tag{12.19}$$

Here $I(\mathcal{T}_\pm)$ is considered a functional of $\mathcal{T}_\pm$ and is defined by

$$I(\mathcal{T}_\pm) = \lim_{F'\to F}\int_{E_a}^{E_b}\int \bar{v}_+(E,\alpha|F',\beta')(H^E-F)v_-(E,\alpha|F,\beta)d\alpha dE \tag{12.20}$$

where

$$v_\pm(E,\alpha|F,\beta) = \delta(E-F)\delta(\alpha,\beta) + \varepsilon\gamma_\pm(F-E)\mathcal{T}_\pm(E,\alpha|F,\beta) \tag{12.21}$$

or equivalently

$$v_\pm(E,\alpha|F,\beta) = u_\pm(E,\alpha|F,\beta) + \varepsilon\gamma_\pm(F-E)\left[\mathcal{T}_\pm(E,\alpha|F,\beta) - T_\pm(E,\alpha|F,\beta)\right]. \tag{12.22}$$

The functions $\mathcal{T}_\pm$ are trial functions which approximate $T_\pm$.

We shall prove that variations of $A(\mathcal{T}_\pm)$ resulting from variations of $\mathcal{T}_\pm$ about $T_\pm$ vanish. Hence $A(\mathcal{T}_\pm)$ is an insensitive functional with respect to $\mathcal{T}_\pm$ in the vicinity of $\mathcal{T}_\pm = T_\pm$ and we can write as an approximation

$$A(\mathcal{T}_\pm) \tilde{=} A(T_\pm) \tag{12.23}$$

where $\widetilde{\mathcal{T}}_{\pm}$ approximates $T_{\pm}$. It will also be shown that

$$I(T_{\pm}) = 0. \tag{12.24}$$

Hence relation (12.23) means

$$A(\widetilde{\mathcal{T}}_{\pm}) \cong \varepsilon\, T_{-}(F,\beta'|F,\beta). \tag{12.25}$$

Relation (12.25) is the one we shall use. From the trial functions $\widetilde{\mathcal{T}}_{\pm}$ in the left hand side of (12.25) we can obtain a more accurate expression for $T_{-}(F,\beta'|F,\beta)$.

The variational principle and equation (12.24) are proved in Appendix III.

It should be noted that in the expression (12.20) for I it is necessary to evaluate the integral before taking the indicated limit. If one takes the limit first, i.e., sets F' equal to F in the integrand, the integrand is not defined because one has the product of two symbolic functions, namely, $v_{+}v_{-}$, which have the same arguments in terms of the variables E and F. Products of symbolic functions having the same arguments are not defined in general. For example, $(\delta(x))^2$ is not defined, though the product $\delta(x)\delta(y)$ is defined. After some manipulation it is possible to break up the integrand into a sum of terms such that terms involving products of symbolic functions are isolated. The integral over these products can be evaluated and the limit $F' \to F$ is then taken. For the remaining terms it is proper to interchange the integration and limiting processes. The procedure discussed is illustrated in the proof of the variational principle (Appendix I).

While the expressions (12.19) through (12.22), which define $A(\mathcal{T}_{\pm})$, are useful in proving the variational principle, an expression more convenient for actual calculations is derived in Appendix IV and is

(12.19a)
$$A(\mathcal{T}_{\pm}) = \varepsilon V^{E}(F,\beta'|F,\beta) + \varepsilon^{2}\left[\int_{E_a}^{E_b}\int \bar{\mathcal{T}}_{+}(E,\alpha|F,\beta')\gamma_{-}(F-E)V^{E}(E,\alpha|F,\beta)\,d\alpha dE + \int_{E_a}^{E_b}\int V^{E}(F,\beta'|E,\alpha)\gamma_{-}(F-E)\mathcal{T}_{-}(E,\alpha|F,\beta)\,d\alpha dE - \int_{E_a}^{E_b}\int \bar{\mathcal{T}}_{+}(E,\alpha|F,\beta')\gamma_{-}(F-E)\mathcal{T}_{-}(E,\alpha|F,\beta)\,d\alpha dE\right] + \varepsilon^{3}\int_{E_a}^{E_b}\int\int_{E_a}^{E_b}\int \bar{\mathcal{T}}_{+}(E,\alpha|F,\beta')\gamma_{-}(F-E)V^{E}(E,\alpha|E',\alpha')\gamma_{-}(F-E') \cdot \mathcal{T}_{-}(E',\alpha'|F,\beta)\,d\alpha' dE' d\alpha dE \,.$$

We can now consider some results. If we take as trial functions $\mathcal{T}_{\pm} = 0$, we find from (12.25) and (12.19a) that we have

$$T_{-}(F,\beta'|F,\beta) \cong V^{E}(F,\beta'|F,\beta)$$

which is just the result one would obtain for $T_{-}(F,\beta'|F,\beta)$ using the first Born approximation. If one chooses for the trial functions the first Born approximation to $T_{\pm}(E,\alpha|F,\beta)$, namely,

(12.26)
$$\mathcal{T}_{\pm}(E,\alpha|F,\beta) = V^{E}(E,\alpha|F,\beta)$$

one sees from the variational principle that one has

$$(12.27)\quad T_-(F,\beta'|F,\beta) \cong V^E(F,\beta'|F,\beta) + \varepsilon \int_{E_a}^{E_b} V^E(F,\beta'|E,\alpha)\gamma_-(F-E)$$

$$\cdot\, V^E(E,\alpha|F,\beta)d\alpha dE + \varepsilon^2 \int_{E_a}^{E_b}\int\int_{E_a}^{E_b} V^E(F,\beta'|E,\alpha)\gamma_-(F-E)$$

$$\cdot\, V^E(E,\alpha|E',\alpha')\gamma_-(F-E')\; V^E(E',\alpha'|F,\beta)d\alpha' dE' d\alpha dE$$

which is just the third Born approximation to $T_-(F,\beta'|F,\beta)$. Kohn* has indicated generally that if $\mathcal{T}_+(E,\alpha|F,\beta)$ is taken to be the m'th Born approximation to $T_+(E,\alpha|F,\beta)$ and $\mathcal{T}_-(E,\alpha|F,\beta)$ is taken to be the n'th Born approximation to $T_-(E,\alpha|F,\beta)$ then the variational principle gives $T_-(F,\beta'|F,\beta)$ to the (m+n+1) Born approximation. The proof of this statement is straightforward.

13. Transition Probabilities per Unit Time.

What is frequently desired in quantum mechanics are transition probabilities per unit time. The simplest way to describe what is wanted is given in terms of our prototype problem in which we consider a particle scattered by a potential. One could consider an ensemble of identical systems, each system consisting of the particle together with its scattering center. In accordance with the principles of quantum mechanics, each member of such an ensemble would correspond to a possible experiment. One could prescribe the probability distribution in the kinetic energy and direction of the particles at time $t = -\infty$ and ask for the rate of growth of probability that the particle has a different kinetic energy and direction at any time t. This rate of growth of the probability is called the transition probability per unit time, if the original probability

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*W. Kohn, Private Communication.

density has a sharp maximum in the energy and direction. In a statistical sense the transition probability per unit time gives the rate at which particles change their original direction and kinetic energy upon "colliding" with the potential.

We shall now formulate the problem mathematically without reference to the prototype model. We shall prescribe the state $\underline{\Phi}_-$ in the H_o representation, and ask for the rate of change of the probability density associated with the state $\underline{\Phi}(t)$ in the H_o representation.

We represent $\underline{\Phi}_-$ and $\underline{\Phi}(t)$ by

$$\underline{\Phi}_- \underset{E}{\longleftrightarrow} f_-(E,\alpha)$$

$$\underline{\Phi}(t) \underset{E}{\longleftrightarrow} f(E,\alpha;t) \ .$$

Using the eigenfunctions u_- we have

$$f(E,\alpha;t) = \int_{E_a}^{E_b} u_-(E,\alpha|F,\beta) f_-(F,\beta) e^{-iFt} d\beta dF .$$

We wish to obtain $W(E,\alpha;t)$ defined by

$$(13.01) \qquad W(E,\alpha;t) = \frac{d}{dt} |f(E,\alpha;t)|^2$$

$$= -i \int_{E_a}^{E_b} \int_{E_a}^{E_b} \bar{u}_-(E,\alpha|F,\beta) u_-(E,\alpha|F',\beta') \bar{f}_-(F,\beta) f_-(F',\beta') (F'-F)$$

$$\cdot e^{-i(F'-F)t} d\beta' dF' d\beta dF$$

inasmuch as

$$\left(\int_{E_1}^{F_1+\Delta E} \int_{\alpha_1}^{\alpha_1+\Delta\alpha} W(E,\alpha;t) d\alpha dE \right) \Big/ (\underline{\Phi}_-, \underline{\Phi}_-)$$

is the rate of growth at time t of the probability that the particle has the energy H_o between E_1 and $E_1 + \Delta E$ and the direction between α_1 and $\alpha_1 + \Delta\alpha$.

Since we can write

$$F'-F = (F'-E) - (F-E) \tag{13.02}$$

and since

$$(F-E)u_-(E,\alpha|F,\beta) = \varepsilon T_-(E,\alpha|F,\beta) \tag{13.03}$$

we have from (13.01)

$$W(E,\alpha;t) = 2\varepsilon\, \mathrm{Im} \int_{E_a}^{E_b}\int_{E_a}^{E_b} \bar{u}_-(E,\alpha|F,\beta)T_-(E,\alpha|F',\beta') \cdot e^{-i(F'-F)t}\, \bar{f}_-(F,\beta)f_-(F',\beta')d\beta' dF' d\beta dF \tag{13.04}$$

where Im means "imaginary part", i.e., $\mathrm{Im}(x + iy) = y$.

We have been considering $\bar{\Phi}_-$ as being a quadratically integrable state. However, now we shall take $\bar{\Phi}_-$ as an eigenstate of H_o with the eigenvalues E',α' and consider such an eigenstate as having been derived from a proper state by a suitable limiting process. We shall take $\bar{\Phi}_-$ to be an eigenstate of H_o corresponding to the eigenvalues E', α'. Hence

$$f_-(E,\alpha) = \delta(E-E')\delta(\alpha,\alpha'). \tag{13.05}$$

Equation (13.04) becomes

$$W(E,\alpha;t) = 2\varepsilon\, \mathrm{Im}\, \bar{u}_-(E,\alpha|E',\alpha')T_-(E,\alpha|E',\alpha'). \tag{13.06}$$

For simplicity let us assume that $\alpha \neq \alpha'$. We then have from (6.27)

$$\bar{u}_-(E,\alpha|E',\alpha') = \varepsilon\bar{\gamma}_-(E'-E)\bar{T}_-(E,\alpha|E',\alpha'). \tag{13.07}$$

It then follows that

$$\bar{u}_-(E,\alpha|E',\alpha')T_-(E,\alpha|E',\alpha') = \varepsilon \left[i\pi\delta(E-E') + \frac{P}{E'-E} \right] |T_-(E,\alpha|E',\alpha')|^2$$

and hence that

$$\mathrm{Im}\ \bar{u}_-(E,\alpha|E',\alpha')T_-(E,\alpha|E',\alpha') = \varepsilon\pi\delta(E-E')\ |T_-(E,\alpha|E',\alpha')|^2 .$$

Upon substitution of this expression into (13.06) we obtain finally

$$W(E,\alpha;t) = 2\pi\varepsilon^2\delta(E-E')\ |T_-(E,\alpha|E',\alpha')|^2 \tag{13.08}$$

which is the expression given, for example, by Lippmann and Schwinger (ref. 6). These authors, however, obtain this result in a more cumbersome manner, largely because they substitute (13.05) into (13.01) prematurely.

It is to be noted that the rate of growth of probability given by (13.08) is independent of the time. Hence the probability of finding a particle with the energy E and direction α increases indefinitely. This result is contrary to the conservation of the probability and is due to our having used an improper state for $\bar{\Phi}_-$. We may follow Friedrichs (ref. 16) and instead of taking $\bar{\Phi}_-$ to be an eigenstate of H_o, we take it to be a proper state such that its H_o representer $f_-(E,\alpha)$ has a sharp peak at $E = E'$, $\alpha = \alpha'$. We shall assume for simplicity that α' is some distance from α which appears as an argument in $W(E,\alpha;t)$. Hence we can use equation (13.07) for $\bar{u}_-$.

We shall further assume that $T_-(E,\alpha|F,\beta)$ and $\frac{P}{F-E}\ T_-(E,\alpha|F,\beta)$ are relatively insensitive functions of the arguments F and β in the vicinity of $F = F'$ and $\beta = \alpha'$ and hence that

$$T_-(E,\alpha|F,\beta)f_-(F,\beta) = T_-(E,\alpha|E',\alpha')\ f_-(F,\beta) \tag{13.09}$$

$$\frac{P}{F-E}T_-(E,\alpha|F,\beta)f_-(F,\beta) = \frac{P}{E'-E}\ T_-(E,\alpha|E',\alpha')f_-(F,\beta). \tag{13.10}$$

Equation (13.04) then becomes

$$(13.11)\quad W(E,\alpha;t) = 2\varepsilon^2 \mathrm{Im} \int_{E_a}^{E_b} \iint_{E_a}^{E_b} i\pi\delta(E-F)\overline{T}_-(E,\alpha|F,\beta)T_-(E,\alpha|F',\beta')$$

$$\cdot e^{-i(F'-F)t}\, \overline{f}_-(F,\beta)f_-(F',\beta')d\beta' dF' d\beta dF$$

$$+ 2\varepsilon^2\, \mathrm{Im} \int_{E_a}^{E_b} \iint_{E_a}^{E_b} \frac{\overline{T}_-(E,\alpha|F,\beta)}{F-E}\; T_-(E,\alpha|F'\beta')\overline{f}_-(F,\beta)\overline{f}_-(F',\beta')$$

$$\cdot e^{-i(F'-F)t}\, d\beta' dF' d\beta dF$$

$$= 2\pi\, \varepsilon^2 \mathrm{Re}\; |T_-(E,\alpha|E',\alpha')|^2 \int_{E_a}^{E_b} \iint e^{-i(F'-E)t}\, \overline{f}_-(E,\beta)f_-(F',\beta')d\beta' d\beta dF'$$

$$+ 2\varepsilon^2\, \mathrm{Im}\, \frac{P}{E'-E} |T_-(E,\alpha|E',\alpha')|^2 \Big| \int_{E_a}^{E_b} f_-(F,\beta)e^{-iFt} d\beta dF \Big|^2 .$$

In the above Re means "real part". Since the imaginary part of the second term is zero, equation (13.11) becomes

$$(13.12)\quad W(E,\alpha;t) = 2\pi\varepsilon^2\, \mathrm{Re}|T_-(E,\alpha|E',\alpha')|^2\, \overline{h}(E) \int_{E_a}^{E_b} e^{-i(F'-E)t}\, h(F')dF'$$

where

$$(13.13)\qquad h(E) = \int f_-(E,\alpha)d\alpha .$$

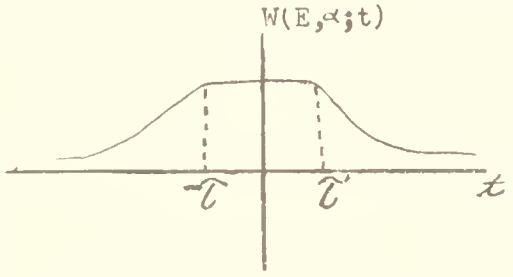
It is noted that if we substitute the eigenstate (13.05) for $f_-(E,\alpha)$, we get our previous result (13.08).

Using the proper state $\overline{\Phi}_-$ we have as a consequence of the Riemann-Lesbegue theorem

$$(13.14)\qquad \lim_{t \to \pm\infty} W(E,\alpha;t) = 0$$

which we desire in order to assure ourselves that the probability does not grow indefinitely as $t \to \pm\infty$. Note also that, because of the appearance of $\bar{h}(E)$ in (13.12), $W(E,\alpha;t)$ is zero unless E is near E'.

It is clear that if $|t|$ is sufficiently small, $|t| < \tau$ say, $W(E,\alpha;t)$ is approximately constant in time. The time τ depends upon the width of the peak about E' of the function $f_-(E,\alpha)$. For fixed values of E,α,E',α' one can expect $W(E,\alpha;t)$ to have the behaviour illustrated below.



A useful "transition lifetime" can be defined as a period of time during which the transition takes place at the approximately constant rate and would be, accordingly, 2τ.

To see how τ depends on the width of the peak of $f_-(E,\alpha)$ or equivalently of $h(E)$ as a function of E, let us take $h(E)$ to be a pulse function defined in the following way:

$$h(E) = K, \qquad E' \le E \le E' + \delta E, \tag{13.15}$$

$$h(E) = 0, \qquad \text{for all other values of } E.$$

Then

$$W(E,\alpha;t) = -2\pi\varepsilon^2 \,\mathrm{Im}\,\frac{K}{t}\,|T_-(E,\alpha|E',\alpha')|^2\,\bar{h}(E)e^{i(E-E')t}\left[e^{-it\delta E} - 1\right]. \tag{13.16}$$

In order to have $W(E,\alpha;t)$ near its maximum, the time t must be smaller than τ where

$$\tau\,\delta E < 1 \tag{13.17}$$

$$\tau(E-E') < 1. \tag{13.18}$$

With these conditions, the exponentials in (13.16) may be expanded in terms of their arguments and the lowest non-vanishing term yields the "constant" part of $W(E,\alpha;t)$, namely,

$$W(E,\alpha;0) = 2\pi\varepsilon^2 |h(E)|^2 \, |T_-(E,\alpha|E',\alpha')|^2 \, \delta E.$$

Condition (13.18) is included in condition (13.17), since for non-vanishing $W(E,\alpha;t)$ we must have

$$0 \leq (E-E') \leq \delta E \tag{13.19}$$

which, when substituted into (13.18) gives (13.17). Condition (13.17) is then the relation between the lifetime of the state and of the uncertainty of the energy measurement of the initial state. It is, in fact, the Heisenberg uncertainty principle (it should be remembered that we have taken $\hbar = 1$). It is in contexts of this character that the Heisenberg uncertainty principle plays its essential role. For a more detailed discussion of the above considerations one may consult reference 16.

14. Adiabatic Switch-on of the Perturbation and the Adiabatic Theorem.

It has been shown that for a large class of solutions

$$\underline{\Phi}(t) = e^{-iHt} \underline{\varphi}(0) \tag{14.01}$$

of the Schroedinger equation (1.01), one can evaluate the limits

$$\lim_{t \to \pm\infty} e^{iH_0 t} \underline{\Phi}(t) = \underline{\Phi}_{\pm} \tag{14.02}$$

Such solutions satisfy the unperturbed Schroedinger equation asymptotically as $t \to \pm\infty$ as pointed out in section 1. The solutions thus behave as though the perturbation had been "switched off" as $t \to \pm\infty$. In particular it was shown by means of the eigenfunctions u_- that if the initial condition on the solution of the Schroedinger equation (1.01) were that the H_0 representer $f(E,\alpha;t)$ should behave like $e^{-iEt} f_-(E,\alpha)$ as $t \to -\infty$, then at finite times the H representer $g(F,\beta;t)$ was given by

$$g(F,\beta;t) = e^{iFt} f_-(F,\beta)$$

this condition being, in fact, the condition used to specify u_- completely.

We shall now consider the problem in which the perturbation is "really" switched off at a very slow rate, i.e., adiabatically, as $t \to -\infty$. We shall show that if we prescribe as the initial condition that the solution of the Schroedinger equation shall behave as above as $t \to -\infty$, then at finite times t the H_0 and H representers, $f(E,\alpha;t)$ and $g(F,\beta;t)$, respectively, are the same as those obtained using the eigenfunctions u_- and assuming the perturbation constant in time.

The use of adiabatic switch-off of the perturbation as $t \to -\infty$ is the one used conventionally to solve the Schroedinger equation in the time-dependent approach to scattering problems (see, e.g., ref. 6 and 8), particularly in the recent work in quantum field theory. Though the use of the spectral representation of H, rather than the adiabatic switch-off procedure, has been used by Dirac (ref. 10) and by others in the time-independent formalism (see section 15), the use of the spectral representation of H in the time-dependent formalism originated with Friedrichs (ref. 4). Snyder (ref. 7) appears to have been the first to have discussed the generally assumed equivalence of the adiabatic switch-off procedure and the procedure of using the spectral representation of H. Friedrichs (ref. 17) has also discussed the equivalence of the adiabatic switch-off procedure to the procedure of using the spectral representation but in a more rigorous fashion.

In their discussion of the use of adiabatic switch off, both Snyder and Friedrichs have restricted themselves to the case where the total Hamiltonian at all times has a continuous spectrum only, which coincides with the spectrum of H_0. In our treatment we shall follow more closely the spirit of the work of Lippmann and Schwinger and Fubini (ref. 18)* in which no explicit assumption is made regarding the total Hamiltonian. However, in our discussion we shall try to indicate the conditions which must be satisfied in order to obtain meaningful results.

Accordingly we introduce the Hamiltonian $H_\zeta(t)$ defined by

$$H_\zeta(t) = H_0 + \varepsilon\, e^{\zeta t}\, V \qquad (\zeta > 0) \tag{14.04}$$

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* The author is indebted to Dr. B. Zumino for this reference.

We note that

$$\lim_{t\to-\infty} H_\zeta(t) = H_o \tag{14.05}$$

and

$$\lim_{\zeta\to 0} H_\zeta(t) = H \tag{14.06}$$

Let us denote by $f_\zeta(E,\alpha;t)$ the H_o representer of $\overline{\Phi}_\zeta(t)$ which is a solution of the Schroedinger equation

$$H_\zeta(t)\,\overline{\Phi}_\zeta(t) = i\frac{\partial}{\partial t}\overline{\Phi}_\zeta(t). \tag{14.07}$$

The representer $f_\zeta(E,\alpha;t)$ thus satisfies the equation

$$i\frac{\partial f_\zeta(E,\alpha;t)}{\partial t} = E\,f_\zeta(E,\alpha;t) + \varepsilon\, e^{\zeta t}\int_{E_a}^{E_b}\int V^E(E,\alpha|E',\alpha') \cdot f_\zeta(E',\alpha';t)\,d\alpha'\,dE' \tag{14.08}$$

We take as initial conditions

$$\lim_{t\to-\infty} e^{iEt} f_\zeta(E,\alpha;t) = f_-(E,\alpha) \tag{14.09}$$

where $f_-(E,\alpha)$ is prescribed. Let us write $f_\zeta(E,\alpha;t)$ in terms of $e^{-iEt}f_-(E,\alpha)$ which is the solution of (14.08) if no perturbation were present in terms of an integral operator as follows:

$$f_\zeta(E,\alpha;t) = \int_{E_a}^{E_b}\int w_{\zeta,t}(E,\alpha|E',\alpha')e^{-iE't} f_-(E',\alpha')\,d\alpha'\,dE' \tag{14.10}$$

It is our objective to show that in many cases $w_{\zeta,t}$ becomes the eigenfunction u_- in the adiabatic limit. That is,

$$\lim_{\zeta \to 0} w_{\zeta,t}(E,\alpha|E',\alpha') = u_-(E,\alpha|E',\alpha'). \tag{14.11}$$

We shall then have, as follows from (6.29) and (6.30), the result that $f_o(E,\alpha;t)$ and $e^{-iFt} f_-(F,\beta)$ are the H_o and H representers, respectively, of the solution $\underline{\Phi}(t)$ of the Schroedinger equation

$$H \underline{\Phi}(t) = i \frac{\partial \underline{\Phi}(t)}{\partial t} \tag{14.12}$$

with the initial condition

$$\lim_{t \to -\infty} e^{iH_o t} \underline{\Phi}(t) = \underline{\Phi}_- \underset{E}{\longleftrightarrow} f_-(E,\alpha).$$

This statement is essentially the adiabatic theorem for the continuous spectrum which can be worded as follows: When a perturbation is switched on infinitely slowly, a superposition of eigenstates of the unperturbed Hamiltonian in the infinite past goes over into the identical superposition of corresponding eigenstates of the total Hamiltonian at finite times.

In our discussion it will be convenient to introduce another integral operator with the kernel $v_{\zeta,t}(E,\alpha|E',\alpha')$ defined by

$$v_{\zeta,t}(E,\alpha|E',\alpha') = w_{\zeta,t}(E,\alpha|E',\alpha')\, e^{i(E-E')t} \tag{14.13}$$

Hence

$$e^{iEt} f_\zeta(E,\alpha;t) = \int_{E_a}^{E_b} \int v_{\zeta,t}(E,\alpha|E',\alpha') f_-(E',\alpha')\, d\alpha'\, dE'. \tag{14.14}$$

The initial condition (14.09) can now be interpreted as an initial condition on $v_{\zeta,t}(E,\alpha|E',\alpha')$, namely,

$$\lim_{t \to -\infty} v_{\zeta,t}(E,\alpha|E',\alpha') = \delta(E-E')\delta(\alpha,\alpha'). \tag{14.15}$$

The simplicity of the initial condition on $v_{\zeta,t}$ motivates its introduction in the present context. It should be pointed out that the kernel or matrix

$v_{\zeta,t}(E,\alpha|E',\alpha')$ is just the operator U_+ of Lippmann and Schwinger as expressed in the H_o representation. This operator also appears in Fubini's paper.

Substitution of (14.14) into the differential equation (14.08) for $f_\zeta(E,\alpha;t)$ and the use of the fact that $f_-(E,\alpha)$ is largely arbitrary leads us to the following equation for $v_{\zeta,t}$:

$$\frac{\partial}{\partial t} v_{\zeta,t}(E,\alpha|E',\alpha') = -i\varepsilon \int_{E_a}^{E_b} \int V^E(E,\alpha|E'',\alpha'') e^{[i(E-E'')+\zeta]t} \cdot v_{\zeta,t}(E'',\alpha''|E',\alpha')\, d\alpha''\, dE'' \tag{14.16}$$

or on integration with respect to t and on using the initial condition (14.15) we find

$$v_{\zeta,t}(E,\alpha|E',\alpha') = \delta(E-E')\delta(\alpha,\alpha') - i\varepsilon \int_{-\infty}^{t} dt' \int_{E_a}^{E_b} \int V^E(E,\alpha|E'',\alpha'') \cdot e^{[i(E-E'')+\zeta]t'} v_{\zeta,t'}(E'',\alpha''|E',\alpha')\, d\alpha''\, dE'' . \tag{14.17}$$

Having used our initial condition, we express $v_{\zeta,t}$ in terms of $w_{\zeta,t}$ (eq. (14.13)) and obtain an equation for $w_{\zeta,t}$

$$w_{\zeta,t}(E,\alpha|E',\alpha') = \delta(E-E')\delta(\alpha,\alpha') - i\varepsilon\, e^{-i(E-E')t} \cdot \int_{-\infty}^{t} dt' \int_{E_a}^{E_b} \int V^E(E,\alpha|E'',\alpha'') e^{[i(E-E')+\zeta]t'} \cdot w_{\zeta,t'}(E'',\alpha''|E',\alpha')\, d\alpha''\, dE'' . \tag{14.18}$$

In equation (14.18) let us now integrate the time integral by parts. We obtain

$$(14.19)\quad w_{\zeta,t}(E,\alpha|E',\alpha') = \delta(E-E')\delta(\alpha,\alpha') - \frac{i\varepsilon e^{\zeta t}}{i(E-E')+\zeta}$$

$$\cdot \int_{E_a}^{E_b} V^E(E,\alpha|E'',\alpha'')w_{\zeta,t}(E'',\alpha''|E',\alpha')d\alpha''\,dE''$$

$$+ \frac{i\varepsilon e^{-i(E-E')t}}{i(E-E')+\zeta} \int_{-\infty}^{t} dt' \int_{E_a}^{E_b} V^E(E,\alpha|E'',\alpha'')\, e^{\left[i(E-E')+\zeta\right]t'}$$

$$\cdot \frac{\partial}{\partial t'} w_{\zeta,t'}(E'',\alpha''|E',\alpha')d\alpha''\,dE''$$

Taking the limit as ζ approaches zero, we find

$$(14.20)\quad w_{o,t}(E,\alpha|E',\alpha') = \delta(E-E')\delta(\alpha,\alpha') + \gamma_-(E'-E)\int_{E_a}^{E_b} V^E(E,\alpha|E'',\alpha'')$$

$$\cdot w_{o,t}(E'',\alpha''|E',\alpha')d\alpha''\,dE'' + i\varepsilon e^{-i(E-E')t} \lim_{\zeta\to 0} \frac{1}{i(E-E')+\zeta}$$

$$\cdot \int_{-\infty}^{t} dt' \int_{E_a}^{E_b} V^E(E,\alpha|E'',\alpha'')e^{\left[i(E-E')+\zeta\right]t'} \frac{\partial}{\partial t'} w_{\zeta,t'}(E'',\alpha''|E',\alpha')d\alpha''dE'' .$$

We see that if

$$(14.21)\quad \lim_{\zeta\to 0} \frac{1}{i(E-E')+\zeta} \int_{-\infty}^{t} dt' \int_{E_a}^{E_b} V^E(E,\alpha|E'',\alpha'')e^{\left[i(E-E')+\zeta\right]t'}$$

$$\cdot \frac{\partial}{\partial t'} w_{\zeta,t'}(E'',\alpha''|E',\alpha')d\alpha''dE'' = 0 ,$$

then $w_{o,t}$ satisfies the same integral equation as the eigenfunction u_-. Since the solution of this integral equation can be shown to be unique, we have the result that (14.21) is a necessary and sufficient condition for $w_{o,t}$ to be identical to the eigenfunction u_-. That is, relation (14.21) is a necessary and sufficient condition for the equivalence of the adiabatic switch-off

procedure and the use of the spectral representation of H in the time-dependent formalism in scattering problems. In our treatment (and that of references 6 and 18) no explicit conditions have been put on the total Hamiltonian H. However, condition (14.21) is essentially a condition on the perturbation and hence also on H.

A sufficient condition for the validity of the adiabatic theorem can be seen to be

$$\lim_{\zeta \to 0} \frac{\partial}{\partial t} w_{\zeta,t}(E,\alpha|E',\alpha') = 0 \tag{14.22}$$

since in this case (14.21) is satisfied. We shall now give arguments to indicate that (14.22) and hence the adiabatic theorem is valid in many cases, even when H has point eigenvalues.

From (14.19) it can be shown that $\partial w_{\zeta,t}/\partial t$ satisfies the following equation.

$$\frac{\partial}{\partial t} w_{\zeta,t}(E,\alpha|E',\alpha') = \frac{e}{(E'-E)+i\zeta} \left\{ \zeta e^{\zeta t} \int_{E_a}^{E_b} \int V^E(E,\alpha|E'',\alpha'') \right.$$

$$\cdot w_{\zeta,t}(E'',\alpha''|E',\alpha') d\alpha'' dE'' + i(E-E') e^{-i(E-E')t} \int_{-\infty}^{t} dt' \int_{E_a}^{E_b} \int V^E(E,\alpha|E'',\alpha'')$$

$$\left. \cdot \frac{\partial}{\partial t'} w_{\zeta,t'}(E'',\alpha''|E',\alpha') e^{\left[i(E-E')+\zeta\right]t'} d\alpha'' dE'' \right\}. \tag{14.23}$$

We note that we can write

$$w_{\zeta,t}(E,\alpha|E',\alpha') = \int_{-\infty}^{t} dt' \frac{\partial}{\partial t'} w_{\zeta,t'}(E,\alpha|E',\alpha') + w_{\zeta,-\infty}(E,\alpha|E',\alpha').$$

However, from (14.19) it is clear that

$$w_{\zeta,-\infty}(E,\alpha|E',\alpha') = \delta(E-E')\delta(\alpha,\alpha')$$

so that (14.23) becomes

$$(14.24)\qquad \frac{\partial}{\partial t} w_{\zeta,t}(E,\alpha|E',\alpha') = \frac{\varepsilon e^{\zeta t}}{(E'-E)+i\zeta} \Bigg\{ \zeta\, V^E(E,\alpha|E',\alpha') + \int_{-\infty}^{t} dt' \int_{E_a}^{E_b} \int V^E(E,\alpha|E'',\alpha'') \Big[\zeta + i(E-E')\, e^{[i(E-E')+\zeta](t'-t)} \Big] \cdot \frac{\partial}{\partial t'} w_{\zeta,t'}(E'',\alpha''|E',\alpha') d\alpha'' dE'' \Bigg\} .$$

so that (14.23) becomes

We can solve equation (14.24) by iteration. We find that

$$(14.25)\qquad \frac{\partial}{\partial t} w_{\zeta,t}(E,\alpha|E',\alpha') = \zeta \Bigg[\varepsilon e^{\zeta t} (E'-E+i\zeta)^{-1} V^E(E,\alpha|E',\alpha') + 2\varepsilon^2 e^{2\zeta t} (E'-E+2i\zeta)^{-1} \int_{E_a}^{E_b} \int V^E(E,\alpha|E'',\alpha'')(E'-E''+i\zeta)^{-1} \cdot V^E(E'',\alpha''|E',\alpha') d\alpha'' dE'' + 3\varepsilon^3 e^{3\zeta t} (E'-E+3i\zeta)^{-1} \int_{E_a}^{E_b} \iint_{E_a}^{E_b} \int V^E(E,\alpha|E'',\alpha'')(E'''-E''+i\zeta)^{-1} \cdot V^E(E'',\alpha''|E''',\alpha''')(E'-E'''+2i\zeta)^{-1} V^E(E''',\alpha'''|E',\alpha') \cdot d\alpha'' dE'' d\alpha''' dE''' + \cdots \Bigg]$$

If the series with the square brackets converges as ζ approaches zero, then it is clear that (14.22) is satisfied. Now when $\zeta \to 0$ the series in brackets is within a factor ε the derivative with respect to ε of the series (11.01) for u_-. Hence if the series for u_- converges, i.e., if u_- is an analytic function in ε, the series in brackets will converge, since the derivative of an analytic function is also analytic and hence is representable as a power series with the same radius of convergence. We thus come to the conclusion that a sufficient condition for the validity of the adiabatic theorem is the convergence of the power series in ε for u_-. Since there are examples

in which the series for u_- converges even when H has point eigenvalues (see e.g., ref. 4) we have indicated that there are cases even when the spectrum of H differs from that of H_o where the adiabatic theorem holds.

We could have obtained the above result by solving equation (14.18) directly by iteration and then allowing ζ to approach zero. We would then have found that the series expression for $w_{o,t}$ is identical to that for u_-. This procedure is, in fact, used by Snyder (ref. 7) in his discussion of the "irrelevelence of the adiabatic theorem". However, it appeared to us useful to indicate explicit conditions, namely, (14.21) or (14.22) under which the adiabatic theorem will hold.

It might be noted that the convergence of the power series for u_- is a sufficient condition only, so that it is possible that the adiabatic theorem will hold even when such a series expansion is not valid. This appears to be the main point of Snyder's treatment in which he assumes $H_\zeta(t)$ has the same spectrum as H_o for all values of ζ and t.

15. The $\underset{\sim}{x}$ Representation and the Time-Independent Approach to Scattering.

Our discussion is thus far independent of the $\underset{\sim}{x}$ representation. However, for scattering problems of the sort usually discussed in atomic theory the perturbations are given in terms of the $\underset{\sim}{x}$ representation, and it thus has become customary to work in this representation, even though it is often easier to formulate the problem in the H_o representation. It is also conventional, when working in the $\underset{\sim}{x}$ representation, to use the time-independent approach to scattering. In the time-independent approach, one looks for eigenfunctions of the total Hamiltonian H in terms of the $\underset{\sim}{x}$ representation. The eigenfunctions of the continuous spectrum are not unique, but they are chosen by requiring that when the distance of the scattered particle from the scattered is great, each eigenfunction approaches a sum of an "incoming wave" which is an eigenfunction of H_o and of "scattered" waves which are outgoing spherical waves in character. Hence, instead of determining the eigenfunctions in terms of the time-dependent procedure, that is, by imposing initial conditions in time upon the solutions of the Schroedinger equation, one imposes boundary conditions in space on the eigenfunctions as given in the $\underset{\sim}{x}$ representation. In what follows we shall

show the equivalence of the eigenfunctions obtained by the time-dependent formalism which we have considered up to now, and those found by the time-independent formalism.

We shall show the equivalence in two cases. In the first case we shall consider our prototype problem which is the scattering of a particle by a potential, and in the second case we shall consider a generalization, namely, the scattering of a particle by a scatterer having internal degrees of freedom, such as a heavy atom. In both cases we shall begin by defining the operators H_o and V and the auxiliary variables α,β.

A. The Scattering of a Particle by a Potential.

In the scattering of a particle by a potential, H_o is taken to be the kinetic energy operator for a single particle, i.e.,

$$H_o^{\underset{\sim}{x}} = \frac{1}{2m} \nabla^2 \tag{15.01}$$

where the superscript $\underset{\sim}{x}$ denotes the operator in the $\underset{\sim}{x}$ representation. The perturbation εV is identified with the scattering potential. The perturbation will be taken to be a function of the position vector $\underset{\sim}{x}$ when it is given in the $\underset{\sim}{x}$ representation

$$V^{\underset{\sim}{x}} = V(\underset{\sim}{x}). \tag{15.01a}$$

The potential $V(\underset{\sim}{x})$ is assumed to decrease more rapidly than the Coulomb potential for large values of $|\underset{\sim}{x}|$.

Let us consider the H_o representation. With our choice of H_o the quantum variable E has the range from 0 to ∞. The quantum variables α are taken to be the polar angles θ, ϕ which give the direction of the momentum. The angle θ is the angle between the momentum vector and the z-axis, while the angle ϕ is the angle which the projection of the momentum vector on the x-y plane makes with the x-axis.

Another way of expressing the H_o representation is in terms of the momentum operators. This representation is convenient because the eigenfunctions of H_o are more simply expressed in terms of the momentum operators. Let us denote the momentum vector by $\underset{\sim}{p}$ with $E = \frac{p^2}{2m}$. Then if the momentum

representer of a state is denoted by $f(\underset{\sim}{p})$, the energy representer of the same state $f(E,\theta,\phi)$ is related to the momentum representer by

$$(15.02) \qquad f(E,\theta,\phi) = (2m^3E)^{1/4}(\sin\theta)^{1/2}\, f(\underset{\sim}{p})$$

where we replace p_x, p_y, p_z by $\sqrt{2mE}\ \sin\theta\cos\phi$, $\sqrt{2mE}\ \sin\theta\sin\phi$ and $\sqrt{2mE}\cos\theta$ respectively, in the right hand side of (15.02). We use the same letter to designate the representers of both the H_o and momentum representations. However, the different arguments serve to distinguish the representers in the two representations.

The relation (15.02) assures us that inner products have the same value in both the H_o and momentum representations, i.e.,

$$(15.03) \qquad \int_0^\infty\int_0^\pi\int_0^{2\pi} \bar{f}^{(1)}(E,\theta,\phi)f(E,\theta,\phi)\,d\phi\,d\theta\,dE = \int \bar{f}^{(1)}(\underset{\sim}{p})f(\underset{\sim}{p})\,d\underset{\sim}{p}$$

where f, $f^{(1)}$ are the representers of the two states $\bar{\Phi}$, and $\bar{\Phi}^{(1)}$, respectively. The integration over $\underset{\sim}{p}$ means integration with respect to the three components of the momentum.

Just as we introduced the matrix of an operator in the H_o representation we can introduce the matrix of an operator in the momentum representation by

$$\bar{\Phi} \underset{\underset{\sim}{p}}{\longleftrightarrow} f(\underset{\sim}{p})$$

$$K\bar{\Phi} \underset{\underset{\sim}{p}}{\longleftrightarrow} \int K^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{p}')f(\underset{\sim}{p}')\,d\underset{\sim}{p}'$$

where $\underset{\underset{\sim}{p}}{\longleftrightarrow}$ denotes the correspondence between an abstract state and its momentum representer. The matrix $K^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{p}')$ is related to the matrix $K^E(E,\theta,\phi|E',\theta',\phi')$ by

$$(15.04) \qquad K^E(E,\theta,\phi|E',\theta',\phi') = (2m^3E)^{1/4}(\sin\theta)^{1/2}(2m^3E')^{1/4}(\sin\theta')^{1/2}K^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{p}')$$

where E, θ are associated with $\underset{\sim}{p}$ and E', θ' are associated with $\underset{\sim}{p}'$. In particular the identity operator yields

$$\delta(E-E')\delta(\theta-\theta')\delta(\phi-\phi') = (2m\,E)^{1/2}\sin\theta\;\delta(\underset{\sim}{p}-\underset{\sim}{p}')\ . \tag{15.05}$$

We shall denote by $\chi_0(\underset{\sim}{x}|E,\theta,\phi)$ the eigenfunctions $\omega_0(E,\theta,\phi)$ of the operator H_0 as given in the $\underset{\sim}{x}$ representation. The eigenfunctions $\chi_0(\underset{\sim}{x}|E,\theta,\phi)$ relate the $\underset{\sim}{x}$ representer of a state to the H_0 representer. Thus if $\Psi(\underset{\sim}{x})$ is the $\underset{\sim}{x}$ representer of $\overline{\Phi}$ and $f(E,\theta,\phi)$ is the H_0 representer, we have

$$\Psi(\underset{\sim}{x}) = \int_0^\infty\int_0^\pi\int_0^{2\pi}\chi_0(\underset{\sim}{x}|E,\theta,\phi)f(E,\theta,\phi)d\phi d\theta dE. \tag{15.06}$$

These eigenfunctions can be given explicitly in terms of the eigenfunctions $\chi_0(\underset{\sim}{x}|\underset{\sim}{p})$ which are the eigenfunctions as given in terms of the momentum variables.

$$\chi_0(\underset{\sim}{x}|\underset{\sim}{p}) = (2\pi)^{-3/2}e^{i(\underset{\sim}{p}\underset{\sim}{x})} \tag{15.07}$$

where $(\underset{\sim}{p}\underset{\sim}{x})$ is the inner product of the vectors $\underset{\sim}{p}$ and $\underset{\sim}{x}$. According to (15.02)

$$\chi_0(\underset{\sim}{x}|E,\theta,\phi) = (2m^3E)^{1/4}(\sin\theta)^{1/2}\,\chi_0(\underset{\sim}{x}|\underset{\sim}{p}). \tag{15.08}$$

We ought to note that $\chi_0(\underset{\sim}{x}|\underset{\sim}{p})$ and $\chi_0(\underset{\sim}{x}|E,\theta,\phi)$ satisfy the following orthogonality relations.

$$\begin{cases}\int\overline{\chi}_0(\underset{\sim}{x}|\underset{\sim}{p})\,\chi_0(\underset{\sim}{x}|\underset{\sim}{p}')d\underset{\sim}{x} = \delta(\underset{\sim}{p}-\underset{\sim}{p}') \\ \int\overline{\chi}_0(\underset{\sim}{x}|\underset{\sim}{p})\,\chi_0(\underset{\sim}{x}'|\underset{\sim}{p})d\underset{\sim}{p} = \delta(\underset{\sim}{x}-\underset{\sim}{x}')\end{cases} \tag{15.09}$$

$$\begin{cases}\int\overline{\chi}_0(\underset{\sim}{x}|E,\theta,\phi)\,\chi_0(\underset{\sim}{x}|E',\theta',\phi')d\underset{\sim}{x} = \delta(E-E')\delta(\theta-\theta')\delta(\phi-\phi') \\ \int_0^\infty\int_0^\pi\int_0^{2\pi}\overline{\chi}_0(\underset{\sim}{x}|E,\theta,\phi)\,\chi_0(\underset{\sim}{x}'|E,\theta,\phi)d\phi d\theta dE = \delta(\underset{\sim}{x}-\underset{\sim}{x}').\end{cases} \tag{15.09a}$$

Now let us consider the H representation and in particular the continuous spectrum of H. Since we have assumed that the continuous spectrum

of H is the same as that of H_o, in the continuum the quantum variable F has the range from zero to ∞. The quantum variables corresponding to β are denoted by ω,ν which have the same range as θ and ϕ respectively. The variables ω,ν are not the directions of the momentum in the ordinary sense, but such variables must exist since we have assumed that H and H_o have the same continuous spectrum which means that both of the spectra have the same multiplicity. We can also introduce a quantity analogous to the momentum vector $\underset{\sim}{p}$ of the free particle. We denote this new vector by $\underset{\sim}{k}$. The quantum variable F is related to $\underset{\sim}{k}$ by $F = \frac{\underset{\sim}{k}^2}{2m}$. The angles ω and ν give the direction of the vector $\underset{\sim}{k}$. If $g(\underset{\sim}{k})$ is the representer of a state $\bar{\Phi}$ in the $\underset{\sim}{k}$ representation, then the representer of $\bar{\Phi}$ in the H representation $g(F,\omega,\nu)$ is related to $g(\underset{\sim}{k})$ by

$$g(F,\omega,\nu) = (2m^3F)^{1/4} (\sin\omega)^{1/2} g(\underset{\sim}{k}) \tag{15.02a}$$

in analogy to (15.02).

Let us denote the $\underset{\sim}{x}$ representers of the eigenfunctions of H by $\chi(\underset{\sim}{x}|F,\omega,\nu)$ and $\chi(\underset{\sim}{x}|k)$ where

$$\chi(\underset{\sim}{x}|F,\omega,\nu) = (2m^3F)^{1/4} (\sin\omega)^{1/2} \chi(\underset{\sim}{x}|\underset{\sim}{k}). \tag{15.08a}$$

The scattering problem usually discussed is the problem of finding $\chi(\underset{\sim}{x}|\underset{\sim}{k})$ or equivalently $\chi(\underset{\sim}{x}|F,\omega,\nu)$ for the continuous spectrum which can be written as the sum of an incident wave and a scattered wave. As mentioned above this formalism, in contrast to that used earlier in our discussion, is time-independent but we shall show its equivalence to the time-dependent formalism.

According to the time-independent formalism we prescribe $\chi(\underset{\sim}{x}|\underset{\sim}{k})$ as being a solution of

$$H^{\underset{\sim}{x}} \chi(\underset{\sim}{x}|\underset{\sim}{k}) = F\chi(\underset{\sim}{x}|\underset{\sim}{k}) \tag{15.10}$$

$$F = \frac{\underset{\sim}{k}^2}{2m} \tag{15.11}$$

or equivalently

$$(15.12) \qquad \left(\frac{k^2}{2m} + \frac{1}{2m} \nabla^2 \right) \chi(\underset{\sim}{x}|\underset{\sim}{k}) = \varepsilon V(\underset{\sim}{x}) \chi(\underset{\sim}{x}|\underset{\sim}{k})$$

subject to the boundary conditions that it be the sum of an incident wave $\chi_o(\underset{\sim}{x}|\underset{\sim}{k})$, which is a solution of

$$(15.13) \qquad \left(\frac{k^2}{2m} + \frac{1}{2m} \nabla^2 \right) \chi_o(\underset{\sim}{x}|\underset{\sim}{k}) = 0$$

and an outgoing spherical wave. Accordingly the solution of (15.12) is

$$(15.14) \qquad \chi(\underset{\sim}{x}|\underset{\sim}{k}) = \chi_o(\underset{\sim}{x}|\underset{\sim}{k}) - \frac{\varepsilon m}{2\pi} \int \frac{e^{i|\underset{\sim}{k}|\,|\underset{\sim}{x} - \underset{\sim}{x}'|}}{|\underset{\sim}{x} - \underset{\sim}{x}'|} V(\underset{\sim}{x}') \chi(\underset{\sim}{x}'|\underset{\sim}{k})\, d\underset{\sim}{x}'$$

or equivalently from (15.08) and (15.08a)

$$(15.15) \qquad \chi(\underset{\sim}{x}|F,\omega,\nu) = \chi_o(\underset{\sim}{x}|F,\omega,\nu) - \frac{\varepsilon m}{2\pi} \int \frac{e^{i|\underset{\sim}{k}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x} - \underset{\sim}{x}'|} V(\underset{\sim}{x}') \chi(\underset{\sim}{x}'|F,\omega,\nu) d\underset{\sim}{x}' \,.$$

We maintain that the eigenfunction $u_-(E,\theta,\varphi|F,\omega,\nu)$ which we obtained by prescribing initial conditions on the time dependent Schroedinger equation is none other than the H_o representer of $\chi(\underset{\sim}{x}|F,\omega,\nu)$ where $\chi(\underset{\sim}{x}|F,\omega,\nu)$ is the solution of (15.14), that is,

$$(15.16) \qquad u_-(E,\theta,\varphi|F,\omega,\nu) = \int \overline{\chi}_o(\underset{\sim}{x}|E,\theta,\varphi)\, \chi(\underset{\sim}{x}|F,\omega,\nu) d\underset{\sim}{x}$$

or from the orthogonality relations (15.09) we have

$$(15.17) \qquad \chi(\underset{\sim}{x}|F,\omega,\nu) = \int_0^\infty \int_0^\pi \int_0^{2\pi} \chi_o(\underset{\sim}{x}|E,\theta,\varphi) u_-(E,\theta,\varphi\ F,\omega,\nu) d\varphi d\theta dE \,.$$

We shall prove this statement by showing that, as a consequence of the integral equation (6.27, 6.28) for u_-, we obtain the integral equation (15.15) for the function $\chi(\underset{\sim}{x}|F,\omega,\nu)$ as given by (15.17).

We first note that on using (6.27) in (15.17) we have

$$(15.18)\qquad \chi(\underset{\sim}{x}|F,\omega,\nu) = \chi_0(\underset{\sim}{x}|F,\omega,\nu) + \varepsilon \int_0^\infty \int_0^\pi \int_0^{2\pi} \chi_0(\underset{\sim}{x}|E,\theta,\phi)\gamma_-(F-E)T_-(E,\theta,\phi|F,\omega,\nu)d\phi d\theta dE$$

where

$$(15.19)\qquad T_-(E,\theta,\phi|F,\omega,\nu) = \int_0^\infty \int_0^\pi \int_0^{2\pi} V^E(E,\theta,\phi|E',\theta',\phi')u_-(E',\theta',\phi'|F,\omega,\nu) \cdot d\phi' d\theta' dE'$$

since from (2.15) we have

$$(15.20)\qquad V^E(E,\theta,\phi|E',\theta',\phi') = (\omega_0(E,\theta,\phi), V\,\omega_0(E',\theta',\phi')) = \int \bar{\chi}_0(\underset{\sim}{x}|E,\theta,\phi)\, V(\underset{\sim}{x})\, \chi_0(\underset{\sim}{x}|E',\theta',\phi')d\underset{\sim}{x}$$

we obtain on using (15.16) and the orthogonality relations (15.09) for $\chi_0(\underset{\sim}{x}|E,\theta,\phi)$ the important relations

$$(15.21)\qquad T_-(E,\theta,\phi|F,\omega,\nu) = \int \bar{\chi}_0(\underset{\sim}{x}'|E,\theta,\phi)\, V(\underset{\sim}{x}')\, \chi(\underset{\sim}{x}'|F,\omega,\nu)d\underset{\sim}{x}'.$$

Thus the second term on the right hand side of (15.18) becomes, on using (15.21)

$$(15.22)\qquad \int_0^\infty \int_0^\pi \int_0^{2\pi} \chi_0(\underset{\sim}{x}|E,\theta,\phi)\gamma_-(F-E)\, T_-(E,\theta,\phi|F,\omega,\nu)d\phi d\theta dE$$

$$= \int d\underset{\sim}{x}'\, V(\underset{\sim}{x}')\, \chi(\underset{\sim}{x}'|F,\omega,\nu) \int_0^\infty \int_0^\pi \int_0^{2\pi} \bar{\chi}_0(\underset{\sim}{x}'|E,\theta,\phi)\gamma_-(F-E)\chi_0(\underset{\sim}{x}|E,\theta,\phi) \cdot d\phi d\theta dE\,.$$

The integral $\int_0^\infty \int_0^\pi \int_0^{2\pi} \bar{\chi}_0(\underset{\sim}{x}'|E,\theta,\phi)\gamma_-(F-E)\, \chi_0(\underset{\sim}{x}|E,\theta,\phi)d\phi d\theta dE$ is of particular interest because, since $\gamma_-(F-E) = \lim_{\zeta\to 0} \dfrac{1}{F-E+i\zeta}$ is the operator

$\lim_{\zeta\to 0} \frac{1}{F-H_0+i\zeta}$ as given in the H_0 representation, the integral gives this operator in the $\underset{\sim}{x}$ representation as the kernel of an integral operator. This kernel, we shall show, is the Green's function which we want. Upon using (15.07) and (15.08) for $\chi_0(\underset{\sim}{x}|E,\theta,\varphi)$ and performing the angular integrations we find

$$(15.23)\quad \int_0^\infty \int_0^\pi \int_0^{2\pi} \overline{\chi}_0(\underset{\sim}{x}'|E,\theta,\varphi)\gamma_-(F-E)\,\chi_0(\underset{\sim}{x}|E,\theta,\varphi)\,d\varphi\,d\theta\,dE =$$

$$\int_0^\infty \int_0^\pi \int_0^{2\pi} \overline{\chi}_0(\underset{\sim}{x}|E,\theta,\varphi)\gamma_-(F-E)\,\chi_0(\underset{\sim}{x}'|E,\theta,\varphi)\,d\varphi\,d\theta\,dE = \lim_{\zeta\to 0} \frac{-2m}{(2\pi)^2|\underset{\sim}{x}-\underset{\sim}{x}'|}$$

$$\cdot \int_0^\infty \frac{\sin\sqrt{2mE}\,|\underset{\sim}{x}-\underset{\sim}{x}'|}{E-(F+i\zeta)}\,dE\,.$$

We introduce momentum coordinates in the integral by letting

$$(15.24)\qquad |\underset{\sim}{p}| = \sqrt{2mE} \qquad\qquad |\underset{\sim}{k}| = \sqrt{2mF}\,.$$

Making use of the symmetry of the kernel of the integrand in terms of $|\underset{\sim}{p}|$ we have

$$(15.25)\quad \int_0^\infty \int_0^\pi \int_0^{2\pi} \overline{\chi}_0(\underset{\sim}{x}'|E,\theta,\varphi)\gamma_-(F-E)\,\chi_0(\underset{\sim}{x}|E,\theta,\varphi)\,d\varphi\,d\theta\,dE$$

$$= \lim_{\zeta\to 0} \frac{-2m}{(2\pi)^2|\underset{\sim}{x}-\underset{\sim}{x}'|} \int_{-\infty}^{+\infty} \frac{|\underset{\sim}{p}|\sin|\underset{\sim}{p}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}{|\underset{\sim}{p}|^2-(|\underset{\sim}{k}|^2+2mi\zeta)}\,d|\underset{\sim}{p}|$$

$$= \lim_{\zeta\to 0} \frac{-2m}{(2\pi)^2|\underset{\sim}{x}-\underset{\sim}{x}'|} \int_{-\infty}^{+\infty} \frac{|\underset{\sim}{p}|\sin|\underset{\sim}{p}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}{(|\underset{\sim}{p}|-\lambda_1)(|\underset{\sim}{p}|-\lambda_2)}\,d|\underset{\sim}{p}|$$

where

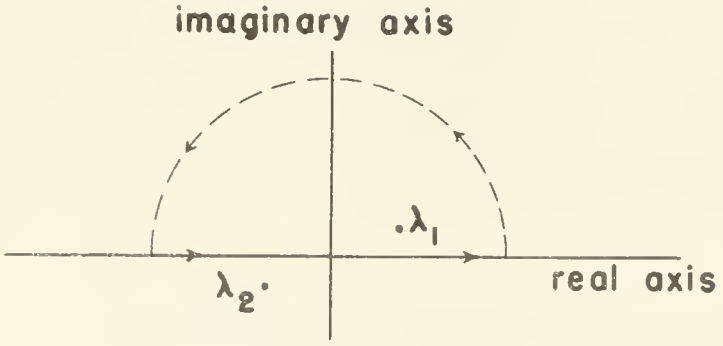
$$(15.26)\qquad \lambda_1 = -\lambda_2 = \left[|\underset{\sim}{k}|^4+4m\zeta^2\right]^{1/4} \exp\frac{i}{2}\left[\tan^{-1}\frac{2m\zeta}{|\underset{\sim}{k}|^2}\right]\,.$$

To evaluate the integral we write

$$(15.27) \qquad \sin|\underset{\sim}{p}|\,|\underset{\sim}{x}-\underset{\sim}{x}'| = \frac{e^{i|\underset{\sim}{p}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|} - e^{-i|\underset{\sim}{p}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}}{2i}$$

Now the integral $\int_{-\infty}^{+\infty} \frac{|\underset{\sim}{p}|\, e^{i|\underset{\sim}{p}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}}{(|\underset{\sim}{p}| - \lambda_1)(|\underset{\sim}{p}| - \lambda_2)}\, d|\underset{\sim}{p}|$

can be found by the integration on the curve formed by the infinite semi-circle on the upper half plane and the real axis as shown below



since the integral vanishes on the semi-circle. By Cauchy's theorem, since the pole λ_1 is enclosed by the contour, we have

$$(15.28) \qquad \lim_{\zeta\to 0}\int_{-\infty}^{+\infty} \frac{|\underset{\sim}{p}|\, e^{i|\underset{\sim}{p}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}}{(|\underset{\sim}{p}|-\lambda_1)(|\underset{\sim}{p}| - \lambda_2)}\, d|\underset{\sim}{p}| = \lim_{\zeta\to 0} \frac{2\pi i\lambda_1\, e^{i\lambda_1|\underset{\sim}{x}-\underset{\sim}{x}'|}}{2\,\lambda_1}$$

$$= i\pi e^{i|\underset{\sim}{k}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}\,.$$

By taking a contour formed by the infinite semi-circle on the lower half plane and the real axis one finds

$$(15.28a) \qquad \lim_{\gamma\to 0}\int_{-\infty}^{+\infty} \frac{|\underset{\sim}{p}| e^{-i|\underset{\sim}{p}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}}{(|\underset{\sim}{p}| - \lambda_1)(|\underset{\sim}{p}| - \lambda_2)}\, d|\underset{\sim}{p}| = -i\pi e^{i|\underset{\sim}{k}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}\,.$$

Hence substituting the above results into (15.25) one finds

$$(15.29)\quad \int_0^{\infty}\int_0^{\pi}\int_0^{2\pi} \overline{\chi_0}(\underset{\sim}{x}'|E,\theta,\phi)\gamma_-(F-E)\,\chi_0(\underset{\sim}{x}|E,\theta,\phi)\,d\phi\,d\Omega\,dE$$

$$= \frac{-4\pi m i}{(2\pi)^2 \cdot 2i\,|\underset{\sim}{x}-\underset{\sim}{x}'|}\, e^{i|\underset{\sim}{k}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|} = -\frac{m}{2\pi}\,\frac{e^{i|\underset{\sim}{k}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x}-\underset{\sim}{x}'|}$$

which is just the Green's function used in the time-independent formalism. The identity (15.29) is a well-known one.

Returning, now, to our expression (15.17) for $\chi(\underset{\sim}{x}|F,\omega,\nu)$ which we have constructed from $u_-(E,\theta,\phi|F,\omega,\nu)$ we find that on using (15.21) and (15.29), and our expression for $\chi(\underset{\sim}{x}|F,\omega,\nu)$ is

$$(15.30)\quad \chi(\underset{\sim}{x}|F,\omega,\nu) = \chi_0(\underset{\sim}{x}|F,\omega,\nu) - \varepsilon\,\frac{m}{2\pi}\int \frac{e^{i|\underset{\sim}{k}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x}-\underset{\sim}{x}'|}\, V(\underset{\sim}{x}')\;\chi(\underset{\sim}{x}'|F,\omega,\nu)\,d\underset{\sim}{x}'$$

which is the same as equation (15.15). Hence we have shown that our eigenfunctions u_- which were specified in terms of initial conditions in time are the eigenfunctions $\chi(\underset{\sim}{x}|F,\omega,\nu)$ which were obtained by specifying boundary conditions in space. It can be shown in a similar way that u_+ corresponds to a solution $\chi(\underset{\sim}{x}|F,\omega,\nu)$ of (15.12) whose scattered part behaves like $\dfrac{e^{-i|\underset{\sim}{k}|\,|\underset{\sim}{x}|}}{|\underset{\sim}{x}|}$ for large $|\underset{\sim}{x}|$.

It is useful to express the amplitude of the spherical wave arising from the second term of (15.30), when $|\underset{\sim}{x}|$ is large, in terms of $T_-(F,\omega,\nu|F,\omega',\nu')$. When $|\underset{\sim}{x}|$ is large, the second term of (15.30) takes the well-known form

$$-\frac{\varepsilon m}{2\pi}\,\frac{e^{i|\underset{\sim}{k}|\,|\underset{\sim}{x}|}}{|\underset{\sim}{x}|}\int e^{-i(\underset{\sim}{k}'\,\underset{\sim}{x}')}\,V(\underset{\sim}{x}')\;\chi(\underset{\sim}{x}'|F,\omega,\nu)\,d\underset{\sim}{x}'$$

where

$$\underset{\sim}{k}' = |\underset{\sim}{k}|\,\frac{\underset{\sim}{x}}{|\underset{\sim}{x}|}$$

Hence using (15.07), (15.08) and (15.21) the amplitude of the spherical wave is

$$\int e^{i(\underset{\sim}{k}' \underset{\sim}{x}')} V(\underset{\sim}{x}') \quad \chi(\underset{\sim}{x}'|F,\omega,\nu)d\underset{\sim}{x}'$$

$$= (2\pi)^{3/2} \int \bar{\chi}_0(\underset{\sim}{x}'|\underset{\sim}{k}') V(\underset{\sim}{x}') \chi(\underset{\sim}{x}'|F,\omega,\nu)d\underset{\sim}{x}' \tag{15.31}$$

$$= (2\pi)^{3/2} (2m^3F)^{-1/4} (\sin \omega')^{-1/2} T_-(F,\omega',\nu'|F,\omega,\nu)$$

where ω,ν give the direction of the incident wave and ω',ν' are the polar angles which give the "direction of observation", i.e., the direction of $\underset{\sim}{x}$. Hence the amplitude of the scattered wave is essentially $T_-(F,\omega',\nu'|F,\omega,\nu)$. This is the result we have obtained also with the scattering operator formalism.

The result takes a somewhat nicer form if we work with the spherical wave associated with the asymptotic form of $\chi(\underset{\sim}{x}|\underset{\sim}{k})$. Then asymptotically

$$\chi(\underset{\sim}{x}|\underset{\sim}{k}) \longrightarrow \chi_0(\underset{\sim}{x}|\underset{\sim}{k}) - \varepsilon m(2\pi)^{1/2} \frac{e^{i|\underset{\sim}{k}| \, |\underset{\sim}{x}|}}{|\underset{\sim}{x}|} T^{\underset{\sim}{p}}_- (\underset{\sim}{k}'|\underset{\sim}{k}) \tag{15.32}$$

$$\underset{\sim}{k}' = |\underset{\sim}{k}| \frac{\underset{\sim}{x}}{|\underset{\sim}{x}|}$$

where $T_-^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{p}')$ is the matrix in the $\underset{\sim}{p}$ representation of the operator whose matrix in the H_0 representation is $T_-^E(E,\theta,\varphi|E',\theta,\varphi') = T_-(E,\theta,\varphi|E',\theta',\varphi')$ or from (15.04)

$$T_-^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{p}') = (2m^3E)^{-1/4} (\sin\theta)^{-1/2} (2m^3E')^{-1/4} (\sin\theta')^{-1/2} \tag{15.33}$$

$$\cdot T_-(E,\theta,\varphi|E',\theta',\varphi')$$

$$= \int \bar{\chi}_0(\underset{\sim}{x}'|\underset{\sim}{p}) V(\underset{\sim}{x}') \quad \chi(\underset{\sim}{x}'|\underset{\sim}{p}') \, d\underset{\sim}{x}'.$$

It is perhaps worthwhile noting that in the $\underset{\sim}{x}$ representation the eigenstates corresponding to one of the point eigenvalues F_i satisfies the integral equation

$$(15.34)\quad \chi(\underset{\sim}{x}|F_i,\beta) = -\frac{\epsilon m}{2\pi}\int \frac{e^{i|\underset{\sim}{k}_i|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x}-\underset{\sim}{x}'|} V(\underset{\sim}{x}')\,\chi(\underset{\sim}{x}'|F_i,\beta)d\underset{\sim}{x}'$$

where

$$|\underset{\sim}{k}_i| = \sqrt{2mF_i}\ .$$

Since $F_i < 0$ we have the result that $i|\underset{\sim}{k}_i|$ is a negative number. Hence when $|\underset{\sim}{x}|$ is large $\chi(\underset{\sim}{x}|F_i, \beta)$ decays exponentially as required.

B. Scattering of a Particle by a System Having Internal Degrees of Freedom.

We wish now to discuss a generalization of the above results, namely, the scattering of a particle by a system having internal degrees of freedom. An example of this situation is the scattering of an electron by an atom. We shall now define H_o and V and indicate the quantum variables. As H_o we take the sum of the kinetic energy operator of the incident particle and the Hamiltonian of the scatterer. The perturbation is taken to be interaction between the incident particle and the scatterer. Let us denote by the subscript 1 the operators associated with the incident particle and by the subscript 2 the operators associated with the scatterer. Then $\underset{\sim}{x}_1$ denotes the set of coordinates of the incident particle and $\underset{\sim}{x}_2$ the coordinates associated with the scatterer. If the scatterer is a heavy atom, $\underset{\sim}{x}_2$ will denote collectively the coordinates which give the position of each of the electrons. We shall assume that in the $\underset{\sim}{x}$ representation the perturbation V is a function of $\underset{\sim}{x}_1$ and $\underset{\sim}{x}_2$

$$V^{\underset{\sim}{x}} = V(\underset{\sim}{x}_1, \underset{\sim}{x}_2)$$

which decays rapidly when $|\underset{\sim}{x}_1|$ is large.

Then the operator H_o is the sum of the operators

$$H_o = T_1 + H_2$$

where T_1 is the kinetic energy operator of the incident particle and H_2 is the Hamiltonian of the scatterer. The total Hamiltonian H is then

$$H = H_o + \varepsilon V = T_1 + H_2 + \varepsilon V. \tag{15.36}$$

We shall now give the nature and ranges of the auxiliary variables α and of E in the spectral representation of H_o. It is clear that the auxiliary variables α will consist of angles Ω, ϕ which give the direction of the incident particle, of the energy of the scatterer, which we denote by E_2, and of the other variables α_2 which together with E_2 give the internal state of the scatterer. The angles Ω,ϕ are just those used in part A of this section and have the same range. The variable E_2 is the quantum number associated with the Hamiltonian H_2 the range of which we take as $E_{20} \leq E_2 \leq E_{21}$. In the case that the scatterer is an atom E_2 would consist of point eigenvalues and a continuum and $E_{21} = +\infty$. We shall, however, not make any explicit assumptions about the spectium of H_2. Furthermore, we shall use the convention that integration over values of E_2 corresponding to point eigenvalues are to be understood as summations. The variable α_2 in the case that the scatterer is an atom might be taken as the variables giving the angular momentum, or when E_2 is in the continuous spectrum, might be used to designate the direction of the ionized electron.

The quantum variable E corresponding to the operator H_o lies in the continuum and has large $E_2 \leq E \leq \infty$. That is, the range of the variable E depends on the auxiliary variable α.

Hence the order of integration is important. For example, if

$$\overline{\Phi} \underset{E}{\longleftrightarrow} f(E,\theta,\phi,E_2,\alpha_2)$$

$$\overline{\Phi}^{(1)} \underset{E}{\longleftrightarrow} f^{(1)}(E,\theta,\phi,E_2,\alpha_2)$$

the inner product $(\underline{\Phi}^{(1)}, \underline{\Phi})$ equals

$$(\underline{\Phi}^{(1)},\underline{\Phi}) = \int_{E_{20}}^{E_{2\perp}} dE_2 \int_{E_2}^{\infty} dE \int_0^{\pi} d\theta \int_0^{2\pi} d\phi \int d\alpha_2 \, \bar{f}^{(1)}(E,\theta,\phi,E_2,\alpha_2)$$

$$\cdot f(E,\theta,\phi,E_2,\alpha_2).$$

The conventional methods of obtaining the eigenfunctions of H is to work in the $\underset{\sim}{x}$ representation and to prescribe suitable boundary conditions in terms of $\underset{\sim}{x}$. We shall sketch the procedure used in reference 3.

First of all, we denote the eigenfunction of the kinetic energy operator T where

$$T^{\underset{\sim}{x}} = -\frac{1}{2m}\nabla^2 \tag{15.37}$$

by $\chi_o(\underset{\sim}{x}|E,\theta,\phi)$ introduced in Part A of this section. The eigenfunctions of H_2 are denoted by $\phi(x_2|E_2,\alpha_2)$. (The function $\phi(\underset{\sim}{x}_2|E_2,\alpha_2)$ is not to be confused with the angle ϕ.) The eigenfunctions of the Hamiltonian H_o corresponding to the total energy E of the unperturbed system, where the free particle has the direction θ,ϕ and the energy and auxiliary variables of the atom have values E_2, α_2 is denoted by $\lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,\theta,\phi,E_2,\alpha_2)$. Clearly

$$\lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,\theta,\phi,E_2,\alpha_2) = \chi_o(\underset{\sim}{x}_1|E-E_2,\theta,\phi)\phi(x_2|E_2,\alpha_2). \tag{15.38}$$

Let us now consider the continuous spectrum of the total Hamiltonian H. Since we have assumed that the continuous spectrum of H is the same as that of H_o, there must be an addition to the quantum variable F variables $\omega, \nu, F_2, \beta_2$ analogous to θ,ϕ,E_2,α_2, respectively. Let us denote the eigenfunctions of H in the $\underset{\sim}{x}$ representation which corresponds to the eigenvalues F and values ω, ν, F_2, β_2 of the variables by $\Psi(\underset{\sim}{x}_1, \underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2)$. Then the equation for $\Psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2)$ is

(15.39) $$H^{\underset{\sim}{x}}\Psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2) = F\,\Psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2)$$

This equation is solved by putting boundary conditions with respect to $\underset{\sim}{x}_1$ on the "mixed" representer of the eigenfunction of H

(15.40) $$F(\underset{\sim}{x}_1|F,\omega,\nu,F_2,\beta_2|E_2,\alpha_2) = \int \varphi(\underset{\sim}{x}_2|E_2,\alpha_2)\,\Psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F_1,\omega,\nu,F_2,\beta_2)\,d\underset{\sim}{x}_2.$$

(The function $F(\underset{\sim}{x}_1|F,\omega,\nu,F_2,\beta_2|E_2,\alpha_2)$ is not to be confused with the quantum variable F).
This mixed representer is the probability amplitude that the scattered particle is in the position $\underset{\sim}{x}_1$ when the scatterer is in the eigenstate described by the quantum variables E_2,α_2. Furthermore, since the effect of the perturbation disappears, when $|\underset{\sim}{x}_1|$ is large, we must have asymptotically

$$\Psi(\underset{\sim}{x}_2,\underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2) \rightarrow \lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2)$$

+ scattered outward spherical waves.

These considerations motivate the boundary conditions on $F(x,|F,\omega,\nu,F_2,\beta_2|E_2,\alpha_2)$ that when $|\underset{\sim}{x}|$ is large, we should have

(15.41) $$F(\underset{\sim}{x}_1|F,\omega,\nu,F_2,\beta_2|E_2,\alpha_2) \rightarrow \chi_0(\underset{\sim}{x}_1|F-F_2,\omega,\nu,)\delta(E_2-F_2)\delta(\alpha_2,\beta_2)$$

+ outward spherical wave in $|\underset{\sim}{x}_1|$

where the δ functions are to be interpreted as Kronecker deltas if the arguments belongs to the discrete spectrum. By substituting

$$\Psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2) = \int_{F_{20}}^{E_{21}}\int F(\underset{\sim}{x}_1|F,\omega,\nu,F_2,\beta_2|E_2,\alpha_2)$$

$$\cdot\ \varphi(\underset{\sim}{x}_2|E_2,\alpha_2)\,d\alpha_2\,dF_2$$

into (15.39) and using the orthogonality properties of $\phi(\underset{\sim}{x}_2|E_2,\alpha_2)$ one obtains a partial differential equation for $F(\underset{\sim}{x}_1|F,\omega,\nu,F_2,\beta_2|E_2,\alpha_2)$ similar in form to equation (15.12) for $\chi(\underset{\sim}{x}|\underset{\sim}{k})$. One then solves for $F(\underset{\sim}{x}_1|F,\omega,\nu,F_2,\beta_2|E_2,\alpha_2)$ using the appropriate Green's function and the incident wave of (15.41). Finally using (15.42) one sees that the eigenfunctions $\Psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2)$ satisfy the integral equation

$$\Psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2) = \lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2)$$

$$(15.43)\qquad -\frac{\varepsilon m}{2\pi}\int_{E_{20}}^{E_{21}}\iiint \frac{e^{i|\underset{\sim}{p}'|\,|\underset{\sim}{x}_1-\underset{\sim}{x}_1'|}}{|\underset{\sim}{x}_1-\underset{\sim}{x}_1'|}\,\phi(\underset{\sim}{x}_2|E_2',\alpha_2')\overline{\phi}(\underset{\sim}{x}_2'|E_2',\alpha_2')$$

$$\cdot\, V(\underset{\sim}{x}_1',\underset{\sim}{x}_2')\;\Psi(\underset{\sim}{x}_1',\underset{\sim}{x}_2'|F,\omega,\nu,F_2,\beta_2)\,d\underset{\sim}{x}_1'\,d\underset{\sim}{x}_2'\,d\alpha_2'\,dE_2'$$

where

$$|\underset{\sim}{p}'| = \sqrt{2m(F-E_2')}$$

In analogy to Part A of this section we assert that $u_-(E,\theta,\phi,E_2,\alpha_2|F,\omega,\nu,F_2,\beta_2)$ obtained by the time dependent formalism is just the H_o representer of the eigenfunction $\Psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2)$. That is,

$$(15.44)\qquad \Psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2)$$

$$=\int_{E_{20}}^{E_{21}} dE_2\int_{E_2}^{\infty} dE\int_0^{\pi} d\theta\int_0^{2\pi} d\phi\int d\alpha_2\;\lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,\theta,\phi,E_2,\alpha_2)$$

$$\cdot\, u_-(E,\theta,\phi,E_2,\alpha_2|F,\omega,\nu,F_2,\beta_2)$$

or equivalently

$$u_-(E,\theta,\phi,F_2,\alpha_2|F,\omega,\nu,F_2,\beta_2)$$

$$(15.44a)\qquad =\iint \bar{\lambda}\,(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,\theta,\phi,E_2,\alpha_2)\;\Psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2)\,d\underset{\sim}{x}_1\,d\underset{\sim}{x}_2\;.$$

As in Part A of this section this assertion is proved by using the integral

equation for u_- in (15.44) and showing that $\Psi(\underset{\sim}{x}_1, \underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2)$ as given by (15.44) satisfies (15.43). The procedure is quite straightforward. The details may be found in reference 19. It is interesting to note that the function generally denoted by $T_-(E,\alpha|F,\beta)$ has the following form in the present case:

(15.45)
$$T_-(E,\theta,\phi,E_2,\alpha_2|F,\omega,\nu,F_2,\beta_2)$$

$$= \int_{E_{20}}^{E_{21}} dE_2' \int_{E_2'}^{\infty} dE' \int_0^{\pi} d\theta' \int_0^{2\pi} d\phi' \int d\ \varepsilon\ V^E(E,\theta,\phi,E_2,\alpha_2|E',\theta',\phi',E_2',\alpha_2')$$

$$\cdot\ u_-(E',\theta',\phi',E_2',\alpha_2'|F,\omega,\nu,F_2,\beta_2)$$

$$= \iint \bar{\lambda}(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,\theta,\phi,E_2,\alpha_2)\ V(\underset{\sim}{x}_1,\underset{\sim}{x}_2)\ \Psi(\underset{\sim}{x}_1,\underset{\sim}{x}_2|F,\omega,\nu,F_2,\beta_2)\, d\underset{\sim}{x}_1 d\underset{\sim}{x}_2$$

where according to equation (2.15)

(15.46)
$$V^E(E,\theta,\phi,E_2,\alpha_2|E_1',\theta',\phi_1',E_2',\alpha_2')$$

$$= \iint \bar{\lambda}\ (\underset{\sim}{x}_1,\underset{\sim}{x}_2|E,\theta,\phi,E_2,\alpha_2)\ V(\underset{\sim}{x}_1,\underset{\sim}{x}_2)\lambda(\underset{\sim}{x}_1,\underset{\sim}{x}_2|E_1',\theta',\phi',E_2',\alpha_2')\, d\underset{\sim}{x}_1, d\underset{\sim}{x}_2 \cdot$$

The asymptotic form of $F(\underset{\sim}{x}_1|F,\omega,\nu,F_2,\beta_2|E_2,\alpha_2)$ which shows how the scattered particle behaves at large distances can be expressed in terms of $T_-(F,\theta,\phi,E_2,\alpha_2|F,\omega,\nu,F_2,\beta_2)$ which is also the amplitude of the scattered wave in the time-dependent formalism. The result is

(15.47)
$$F(\underset{\sim}{x}_1|F,\omega,\nu,F_2,\beta_2|E_2,\alpha_2) \longrightarrow \delta(F_2-E_2)\delta(\alpha_2,\beta_2)\ \chi_0(\underset{\sim}{x}_1|F-F_2,\omega,\nu)$$

$$- \frac{\varepsilon m}{2\pi}\ \frac{e^{i|\underset{\sim}{p}'|\ |\underset{\sim}{x}_1|}}{|\underset{\sim}{x}_1|}\ (2\pi)^{3/2}\ \left[2m^3(F-E_2)\right]^{-1/4}\ (\sin\theta)^{-1/2}$$

$$\cdot\ T_-(F,\theta,\phi,E_2,\alpha_2|F,\omega,\nu,F_2,\beta_2)$$

where $E_2 < F$

$$|\underset{\sim}{p}'| = \sqrt{2m(F-E_2)}$$

and angles θ, φ are the angles giving the direction of observation $\frac{\underset{\sim}{x}_1}{|\underset{\sim}{x}_1|}$.

Hence the amplitude of the outgoing spherical wave is given essentially by $T_-(F,\theta,\varphi,E_2,\alpha_2|F,\omega,\nu,F_2,\beta_2)$.

16. The Time-Independent Definition of the Scattering Operator.

In defining the scattering operator, we have used the time-dependent formalism. The eigenfunctions of H in the $\underset{\sim}{x}$ representation obtained from a time-independent formalism are the same as those obtained from a time-dependent formalism. We shall now show that it is also possible to obtain the scattering operator from a time-independent formalism.

We shall restrict our discussion to the case treated in Part A of Section 15, namely, the scattering of a particle by a potential which decays sufficiently rapidly when $|\underset{\sim}{x}|$ approaches infinity. However, the results can be easily generalized to apply to the case discussed in Part B of Section 15, where a particle is scattered by a center having internal degrees of freedom.

We call our approach time-independent because we shall use the eigenfunctions $\chi(\underset{\sim}{x}|\underset{\sim}{k})$ satisfying equation (15.14) obtained from the time-independent approach. The significance of this approach is due to its connection with the definition of the scattering operator used for the ordinary wave equation. In fact, the method of defining the scattering operator used in this section is analogous to that used, for example, by Friedrichs (ref. 20) for the ordinary wave equation.

We shall consider wave packets, $\Psi(\underset{\sim}{x},t)$, of eigenfunctions, $\chi(\underset{\sim}{x}|k)$, and introduce a moving observer whose velocity is $\underset{\sim}{v}$ and whose position at time t is given by $\underset{\sim}{x} = \underset{\sim}{x}_0 + \underset{\sim}{v}t$. The nature of the function $\Psi(\underset{\sim}{x}_0 + \underset{\sim}{v}t,t)$ as $t \to \pm\infty$ shows what the observer would see for large values of $|\underset{\sim}{x}|$ "before" and "after" the collision. The relationship of $\lim_{t\to+\infty} \Psi(\underset{\sim}{x}_0 + \underset{\sim}{v}t,t)$ to $\lim_{t\to-\infty} \Psi(\underset{\sim}{x}_0 + \underset{\sim}{v}t,t)$ will be used to define the scattering operator.

Before going into detail we shall indicate a useful representation of the δ-function, namely,

$$(16.01)\qquad \lim_{\alpha\to\infty} \alpha^{1/2}\, e^{\pm i\xi^2\alpha} = \pi^{1/2} e^{\pm i\pi/4}\, \delta(\xi).$$

Equation (16.01) is easily proved by evaluating the integral

$$\int_{-\infty}^{+\infty} \alpha^{1/2} e^{\pm i\xi^2\alpha}\, f(\xi)\,d\xi,$$

where $f(\xi)$ is an arbitrary function which vanishes as $\xi \to \pm\infty$ and which is differentiable over the entire range of integration. Integrating by parts, one has

$$(16.02)\qquad \int_{-\infty}^{+\infty} \alpha^{1/2}\, e^{\pm i\xi^2\alpha}\, f(\xi)\,d\xi$$

$$= \left[f(\xi)\alpha^{1/2} \int_{-\infty}^{\xi} e^{i\zeta^2\alpha}\, d\zeta \right]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} d\xi \left[\int_{-\infty}^{\xi} \alpha^{1/2} e^{\pm i\zeta^2\alpha} d\zeta \right] f'(\xi)$$

where $f'(\xi)$ is the derivative of $f(\xi)$. The first term on the right of equation (16.02) vanishes because $f(\pm\infty) = 0$. Let us consider the function $\alpha^{1/2}\int_{-\infty}^{\xi} e^{\pm i\zeta^2\alpha}\, d\zeta$ which appears in the second term. By changing variables this function becomes $\int_{-\infty}^{\xi\alpha^{1/2}} e^{\pm it^2}\, dt$. Now if ξ is negative,

$$\lim_{\alpha\to\infty} \int_{-\infty}^{\xi\alpha^{1/2}} e^{\pm it^2}\, dt = 0 .$$

If ξ is positive,

$$\lim_{\alpha\to\infty} \int_{-\infty}^{\xi\alpha^{1/2}} e^{\pm it^2}\, dt = \int_{-\infty}^{+\infty} e^{\pm it^2}\, dt$$

$$= (1 \pm i)\sqrt{\frac{\pi}{2}} = \sqrt{\pi}\, e^{\pm i\pi/4}$$

or more concisely

$$(16.03)\qquad \lim_{\alpha\to\infty} \int_{-\infty}^{\xi\alpha^{1/2}} e^{\pm it^2}\, dt = \eta(\xi)\sqrt{\pi}\, e^{\pm i\pi/4}$$

where $\eta(\xi)$ is the step function,

$$(16.04)\qquad \eta(\xi) = 0, \quad \xi < 0;$$

$$\eta(\xi) = 1, \quad \xi > 0.$$

Then using (16.04) in equation (16.02)

$$(16.05)\qquad \lim_{\alpha\to\infty} \int_{-\infty}^{+\infty} \alpha^{1/2} e^{\pm i\xi^2\alpha} f(\xi)d\xi = -\int_{0}^{+\infty} f'(\xi)\, d\xi = f(0)$$

since $f(+\infty) = 0$. Inasmuch as $f(\xi)$ is largely arbitrary, equation (16.01) follows. An immediate generalization of (16.01) will also prove useful, namely,

$$(16.06)\qquad \lim_{\alpha\to\infty} \alpha^{3/2}\, e^{\pm i\underset{\sim}{\xi}^2\alpha} = \pi^{3/2}\, e^{\pm i3\pi/4}\, \delta(\underset{\sim}{\xi})$$

where $\delta(\underset{\sim}{\xi})$ is the three dimensional δ-function, which is also given by the product $\delta(\xi_x)\delta(\xi_y)\delta(\xi_z)$, where ξ_x, ξ_y, ξ_z are the cartesian components of the vector $\underset{\sim}{\xi}$.

We now proceed to our objective of defining the scattering operator. A solution of the perturbed Schroedinger equation is the wave packet

$$(16.07)\qquad \Psi(x,t) = \int \chi(\underset{\sim}{x}|\underset{\sim}{k}) e^{-iEt}\, g(\underset{\sim}{k})d\underset{\sim}{k}$$

$$= \int \chi(\underset{\sim}{x}|\underset{\sim}{k}) \exp\left(-i\,\frac{k^2}{2m}\,t\right) g(\underset{\sim}{k})d\underset{\sim}{k}$$

where $\chi(\underset{\sim}{x}|\underset{\sim}{k})$ are the eigenfunctions of H in the $\underset{\sim}{x}$ representation. We shall construct such solutions only of the eigenfunctions of the continuous spectrum of H.

Now from (15.14) we have

$$(16.08)\qquad \chi(\underset{\sim}{x}|\underset{\sim}{k}) = \chi_0(\underset{\sim}{x}|\underset{\sim}{k}) - \frac{\varepsilon m}{2\pi}\,\frac{e^{i|\underset{\sim}{k}|\,|\underset{\sim}{x}|}}{|\underset{\sim}{x}|}\,\zeta(\underset{\sim}{x}|\underset{\sim}{k})$$

where

$$\chi_0(\underset{\sim}{x}|\underset{\sim}{k}) = (2\pi)^{-3/2}\, e^{i(\underset{\sim}{k}\,\underset{\sim}{x})}$$

and

$$(16.09)\qquad \zeta(\underset{\sim}{x}|\underset{\sim}{k}) = |\underset{\sim}{x}| e^{-i|\underset{\sim}{k}|\,|\underset{\sim}{x}|} \int \frac{e^{i|\underset{\sim}{k}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x} - \underset{\sim}{x}'|}\, V(\underset{\sim}{x}')\chi(\underset{\sim}{x}'|\underset{\sim}{k})d\underset{\sim}{x}' \ .$$

From equations (15.32) and (15.33) we have

(16.10)

$$\lim_{|\underset{\sim}{x}|\to\infty} \zeta(\underset{\sim}{x}|\underset{\sim}{k}) = (2\pi)^{3/2} T^{p}_{-}(\underset{\sim}{k}'|\underset{\sim}{k}) = (2\pi)^{3/2} \int \overline{\chi}_{o}(\underset{\sim}{x}'|\underset{\sim}{k}') V(\underset{\sim}{x}') \chi(\underset{\sim}{x}'|\underset{\sim}{k}) d\underset{\sim}{x}'$$

where

$$\underset{\sim}{k}' = |\underset{\sim}{k}| \frac{\underset{\sim}{x}}{|\underset{\sim}{x}|} .$$

We shall now derive an asymptotic form for $\Psi(\underset{\sim}{x}_o + \underset{\sim}{v}t, t)$ as $t \to -\infty$. Such an asymptotic form is obtained by considering the expression for

$$\lim_{t\to-\infty} \left(\sqrt{\frac{-t}{2m}}\right)^3 \exp\left(-i \frac{p_o^2}{2m} t\right) \Psi\left(\underset{\sim}{x}_o + \frac{\underset{\sim}{p}_o}{m} t, t\right)$$

where $\underset{\sim}{p}_o$ is given by $\underset{\sim}{p}_o = m \underset{\sim}{v}$.

We note that

$$(16.11) \quad \left|\underset{\sim}{x}_o + \frac{\underset{\sim}{p}_o}{m} t\right| = \frac{|\underset{\sim}{p}_o|}{m} |t| + \frac{(\underset{\sim}{p}_o \underset{\sim}{x}_o)}{|\underset{\sim}{p}_o|} \operatorname{sgn} t + O\left(\frac{1}{t}\right)$$

where $\operatorname{sgn} t = \frac{t}{|t|}$.

Substituting (16.08) and (16.11) into our expression (16.07) where we take $\underset{\sim}{x} = \underset{\sim}{x}_o + \frac{\underset{\sim}{p}_o}{m} t$ we see that

(16.12)

$$\lim_{t\to-\infty} \left(\sqrt{\frac{-t}{2m}}\right)^3 \exp\left(-i \frac{p_o^2}{2m} t\right) \Psi\left(\underset{\sim}{x}_o + \frac{\underset{\sim}{p}_o}{m} t, t\right) =$$

$$\lim_{t\to-\infty} \left(\sqrt{\frac{-t}{2m}}\right)^3 \int \chi_o(\underset{\sim}{x}_o|\underset{\sim}{k}) \exp\left[-i(\underset{\sim}{k} - \underset{\sim}{p}_o)^2 \left(-\frac{t}{2m}\right)\right] g(\underset{\sim}{k}) d\underset{\sim}{k}$$

$$- \frac{\pi m}{2m} \lim_{t\to-\infty} \frac{\left(-\frac{t}{2m}\right)}{-|\underset{\sim}{p}_o| t - \frac{(\underset{\sim}{p}_o \underset{\sim}{x}_o)}{|\underset{\sim}{p}_o|} + O\left(\frac{1}{t}\right)}$$

$$\cdot \int \Big\{ \lim_{t\to-\infty} \sqrt{\frac{-t}{2m}}\ \exp\left[i(|\underset{\sim}{k}| + |\underset{\sim}{p}_o|)^2 \left(\frac{-t}{2m}\right)\right]$$

$$\cdot \lim_{t\to-\infty} \exp\left[-i|\underset{\sim}{k}|\ \frac{(\underset{\sim}{p}_o \underset{\sim}{x}_o)}{|\underset{\sim}{p}_o|} + i|\underset{\sim}{k}|\ O(\tfrac{1}{t})\right]$$

$$\cdot \lim_{t\to-\infty} \zeta(\underset{\sim}{x}_o + \frac{\underset{\sim}{p}_o}{m} t,\ t)\Big\}\ g(\underset{\sim}{k})d\underset{\sim}{k}\ .$$

We shall now evaluate the right hand side of (16.12). In the first term

(16.13)
$$\lim_{t\to-\infty} \left(\sqrt{\frac{-t}{2m}}\right)^3 \exp\left[i(\underset{\sim}{k}-\underset{\sim}{p}_o)^2 \left(\frac{-t}{2m}\right)\right] = \pi^{3/2}\ e^{i\,3\pi/4}\ \delta(\underset{\sim}{k} - \underset{\sim}{p}_o)$$

as follows from (16.06). Hence the first term is given by

$$\int \chi_o(\underset{\sim}{x}_o|\underset{\sim}{k})\delta(\underset{\sim}{k} - \underset{\sim}{p}_o)g(\underset{\sim}{k})d\underset{\sim}{k} = \pi^{3/2}\ e^{i\,3\pi/4}\ \chi_o(\underset{\sim}{x}_o|\underset{\sim}{p}_o)g(\underset{\sim}{p}_o).$$

To evaluate the second term we note the appearance of the factor

$$\lim_{t\to-\infty} \sqrt{\frac{-t}{2m}}\ \exp\left[i(|\underset{\sim}{k}| + |\underset{\sim}{p}_o|)^2 \left(\frac{-t}{2m}\right)\right].$$

According to (16.01) we have

$$\lim_{t\to-\infty} \sqrt{\frac{-t}{2m}}\ \exp\left[i(|\underset{\sim}{k}| + |\underset{\sim}{p}_o|)^2 \left(\frac{-t}{2m}\right)\right] = \pi^{1/2}\ e^{i\,\pi/4}\ \delta(|\underset{\sim}{k}| + |\underset{\sim}{p}_o|) \equiv 0$$

inasmuch as the argument of the δ-function can never be zero. Hence only the first term on the right of (16.12) survives and we have

(16.15)
$$\lim_{t\to-\infty} \left(\sqrt{\frac{-t}{2m}}\right)^3 \exp\left(-i\,\frac{p_o^2}{2m}\,t\right)\ \Psi(x_o + \frac{p_o}{m}\,t, t)$$
$$= \pi^{3/2}\ e^{i\,3\pi/4}\ \chi_o(\underset{\sim}{x}_o|\underset{\sim}{p}_o)g(\underset{\sim}{p}_o).$$

In a symbolic fashion we may write

(16.15a)
$$\lim_{t\to-\infty} \Psi(\underset{\sim}{x}_o + \frac{\underset{\sim}{p}_o}{m}\,t, t) \cong A(t)\ \chi_o(\underset{\sim}{x}_c|\underset{\sim}{p}_o)g(\underset{\sim}{p}_o)$$

where

$$A(t) = \left(\sqrt{\frac{-t}{2m}}\right)^3 \exp\left(i\frac{p_o^2}{2m}t\right)\pi^{3/2}\, e^{i\,3\pi/4} \quad . \tag{16.15b}$$

Hence, before collision the observer would see (except for the time factor A(t)) only the plane wave component of the wave packet corresponding to the vector $\underset{\sim}{p}_o$ and having the amplitude $g(\underset{\sim}{p}_o)$.

Let us now consider the asymptotic form of $\Psi(\underset{\sim}{x}_o + \frac{\underset{\sim}{p}_o}{m}t, t)$ as $t \to +\infty$. In this case relation (16.12) is replaced by

$$\lim_{t\to+\infty}\left(\sqrt{\frac{t}{2m}}\right)^3 \exp\left(-i\frac{p_o^2}{2m}t\right)\Psi(\underset{\sim}{x}_o + \frac{\underset{\sim}{p}_o}{m}t, t) = \tag{16.16}$$

$$\lim_{t\to+\infty}\left(\frac{t}{2m}\right)^3 \int \chi_o(\underset{\sim}{x}_o|\underset{\sim}{k}) \exp\left[-i(\underset{\sim}{k} - \underset{\sim}{p}_o)^2\left(\frac{t}{2m}\right)\right] g(\underset{\sim}{k})\,d\underset{\sim}{k}$$

$$- \frac{\varepsilon m}{2\pi} \lim_{t\to+\infty} \frac{\frac{t}{2m}}{\frac{|\underset{\sim}{p}_o|}{m}t + \frac{(\underset{\sim}{p}_o\,\underset{\sim}{x}_o)}{|\underset{\sim}{p}_o|} + O\left(\frac{1}{t}\right)} \int \left\{ \lim_{t\to+\infty} \sqrt{\frac{t}{2m}}\, e^{-i(|\underset{\sim}{p}_o| - |\underset{\sim}{k}|)^2\left(\frac{t}{2m}\right)} \right.$$

$$\cdot \lim_{t\to+\infty} \exp\left[i|\underset{\sim}{k}| \frac{(\underset{\sim}{p}_o\,\underset{\sim}{x}_o)}{|\underset{\sim}{p}_o|} + \underset{\sim}{k}\, O\left(\frac{1}{t}\right) \right]$$

$$\left. \cdot \lim_{t\to+\infty} \zeta\left(\underset{\sim}{x}_o + \frac{\underset{\sim}{p}_o}{m}t\,|\underset{\sim}{k}\right) \right\} g(\underset{\sim}{k})\,d\underset{\sim}{k} \quad .$$

In a treatment similar to that for equation (16.12) it can be shown that the first term on the right of (16.15) is $\pi^{3/2}\, e^{-i\,3\pi/4}\, \chi_o(\underset{\sim}{x}_o|\underset{\sim}{p}_o)\, g(\underset{\sim}{p}_o)$. The second term is evaluated by noting the following limits:

$$\lim_{t\to+\infty} \frac{\left(\frac{t}{2m}\right)}{\frac{|\underset{\sim}{p}_o|}{m}t + \frac{(\underset{\sim}{p}_o\,\underset{\sim}{x}_o)}{|\underset{\sim}{p}_o|} + O\left(\frac{1}{t}\right)} = \frac{1}{2|\underset{\sim}{p}_o|} \tag{16.17}$$

$$\lim_{t\to+\infty} \sqrt{\frac{t}{2m}}\, e^{-i(|\underset{\sim}{p}_o| - |\underset{\sim}{k}|)^2\left(\frac{t}{2m}\right)} = \pi^{1/2}\, e^{-i\,\pi/4}\, \delta(|\underset{\sim}{k}| - |\underset{\sim}{p}_o|) \tag{16.18}$$

which follows from (16.01),

$$(16.19)\qquad \lim_{t\to+\infty} \exp\left[i\,|\underset{\sim}{k}|\,\frac{(\underset{\sim}{p}_o\,\underset{\sim}{x}_o)}{|\underset{\sim}{p}_o|} + |\underset{\sim}{k}|\;\;0(\frac{1}{t}) \right]$$

$$= \exp\left[i|\underset{\sim}{k}|\,\frac{(\underset{\sim}{p}_o\,\underset{\sim}{x}_o)}{|\underset{\sim}{p}_o|} \right] = (2\pi)^{3/2}\,\chi_o(\underset{\sim}{x}_o|\underset{\sim}{k}_o)$$

where

$$\underset{\sim}{k}_o = |\underset{\sim}{k}|\,\frac{\underset{\sim}{p}_o}{|\underset{\sim}{p}_o|}$$

$$(16.20)\qquad \lim_{t\to+\infty} \zeta(\underset{\sim}{x}_o + \frac{\underset{\sim}{p}_o\,t}{m}\,,\,\underset{\sim}{k}) = (2\pi)^{3/2}\,T^{\underset{\sim}{p}}_{-}(\underset{\sim}{k}_o|\underset{\sim}{k})$$

which follows from (16.10). On combining all of the above results we find

$$(16.21)\qquad \lim_{t\to+\infty} \left(\sqrt{\frac{t}{2m}}\right)^3 \exp(-i\,\frac{p_o^2}{2m}\,t)\,\Psi(\underset{\sim}{x}_o + \frac{\underset{\sim}{p}_o}{m}\,t,t) = \pi^{3/2}\,e^{-i\,3\pi/4}\,\chi_o(\underset{\sim}{x}_o|\underset{\sim}{p}_o)$$

$$\cdot\left[g(\underset{\sim}{p}_o) - 2\pi i\epsilon m|\underset{\sim}{p}_o|^{-1}\int \delta(|\underset{\sim}{p}_o| - |\underset{\sim}{k}|)T^{\underset{\sim}{p}}_{-}(\underset{\sim}{p}_o|\underset{\sim}{k})\,g(\underset{\sim}{k})d\underset{\sim}{k}\right].$$

One could, of course, eliminate the δ-function by going to spherical coordinates in momentum space. However, for our purpose it is not useful to do this.

We can write (16.21) in a symbolic fashion as

$$(16.22)\qquad \lim_{t\to+\infty} \Psi(\underset{\sim}{x}_o + \frac{\underset{\sim}{p}_o\,t}{m},\,t) \cong A(t)\,\chi_o(\underset{\sim}{x}_o|\underset{\sim}{p}_o)\,g_+(\underset{\sim}{p}_o)$$

where

$$(16.22a)\qquad g_+(\underset{\sim}{p}_o) = g(\underset{\sim}{p}_o) - 2\pi i\epsilon m|\underset{\sim}{p}_o|^{-1}\int \delta(|\underset{\sim}{p}_o| - |\underset{\sim}{k}|)g(k)T^{\underset{\sim}{p}}_{-}(\underset{\sim}{p}_o|\underset{\sim}{k})d\underset{\sim}{k}\,.$$

Hence after collision the observer also sees a plane wave whose direction and wave length are given by $\underset{\sim}{p}_o$. However the amplitude after collision is $g_+(\underset{\sim}{p}_o)$ whereas before collision it was $g(\underset{\sim}{p}_o)$.

We now define the scattering of operator as the operator which relates $g_+(\underset{\sim}{p})$ to $g(\underset{\sim}{p})$. If we write the operator as an integral operator with the "matrix"

$$(16.23)\qquad g_+(\underset{\sim}{p}) = \int S(\underset{\sim}{p}|\underset{\sim}{p}')\,g(\underset{\sim}{p}')d\underset{\sim}{p}'$$

we see

$$(16.24)\quad S(\underset{\sim}{p}|\underset{\sim}{p}') = \delta(\underset{\sim}{p}-\underset{\sim}{p}') - 2\pi i\varepsilon m\,|\underset{\sim}{p}|^{-1}\,\delta(|\underset{\sim}{p}| - |\underset{\sim}{p}'|)T_{-}^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{p}')\ .$$

We maintain that the scattering operator obtained in the time-independent formalism is the same as that obtained using the time-dependent formalism used earlier. To prove this assertion we shall show that $S(\underset{\sim}{p}|\underset{\sim}{p}')$ of equation (16.23) is nothing other than the matrix of the scattering operator the time-dependent formalism when expressed in the momentum representation, i.e.,

$$(16.25)\quad S(\underset{\sim}{p}|\underset{\sim}{p}') = S^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{p}').$$

We note from (15.04) that

$$S^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{p}') = S^{E}(E,\theta,\phi|E',\theta',\phi')(2m^3E)^{-1/4}(\sin\theta)^{-1/2}(2m^3E')^{-1/4}(\sin\theta')^{-1/2}.$$

From the time-dependent definition of $S^{E}(E,\theta,\phi|E',\theta',\phi')$ it follows that

$$(16.26)\quad S^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{p}') = \delta(E-E')\delta(\theta-\theta)\delta(\phi-\phi')\,(2m^3E)^{-1/2}(\sin\theta)^{-1}$$

$$-2\pi i\varepsilon\delta(E-E')T_{-}(E,\theta,\phi|E',\theta',\phi')\,(2m^3E)^{-1/4}(\sin\theta)^{-1/2}(2mE')^{-1/4}(\sin\theta')^{-1/2}\ .$$

However, from (15.05) and (15.33)

$$\delta(E-E')\delta(\theta-\theta')\delta(\phi-\phi')(2m^3E)^{-1/2}(\sin\theta)^{-1} = \delta(\underset{\sim}{p}-\underset{\sim}{p}')$$

and

$$T_{-}(E,\theta,\phi|E',\theta',\phi')(2mE)^{-1/4}(\sin\theta)^{-1/2}(2mE')^{-1/4}(\sin\theta')^{-1/2}$$

$$= T_{-}^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{p}').$$

Furthermore, from the properties of the δ-function

$$\delta(E-E') = \delta\left(\frac{\underset{\sim}{p}^2}{2m} - \frac{\underset{\sim}{p}'^2}{2m}\right) = 2m\delta(\underset{\sim}{p}^2 - \underset{\sim}{p}'^2)$$

$$= m\left[\delta(|\underset{\sim}{p}| - |\underset{\sim}{p}'|) + \delta(|\underset{\sim}{p}| + |\underset{\sim}{p}'|)\right]|\underset{\sim}{p}|^{-1}$$

$$= \frac{m}{|\underset{\sim}{p}|}\delta(|\underset{\sim}{p}| - |\underset{\sim}{p}'|).$$

After making the above substitution in (16.26) one sees that the expression for $S^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{p}')$ is identical to that of $S(\underset{\sim}{p}|\underset{\sim}{p}')$.

17. Definitions of Cross-Section.

In the present section we shall discuss three-possible definitions of cross-sections and show that they give essentially the same result. The first definition—the one conventionally used most—is the time-independent definition and is based on the asymptotic form of the eigenfunction as given in the $\underset{\sim}{x}$ representation. The second definition is based on the use of the scattering operator. The third is based upon the use of time-proportional transition probabilities. Still other definitions are possible, but the three mentioned above seem to be the most useful. We shall restrict our discussion to the case where a particle is scattered by a center of force. However, the discussion can be generalized to include the scattering of a particle by a system having internal degrees of freedom.

A. Time-Independent Definition.

In all the definitions of cross-sections one works with improper eigenfunctions of H of which the incident wave part is an eigenfunction of H_o such that it describes a particle with a definite momentum. The time-independent definition of the differential cross-section is given by

$$(17.01)\quad \sigma(\theta,\varphi)d\Omega = \frac{\text{rate of increase of particles scattered in solid angle } d\Omega}{\text{flux of incident particles through surface normal to momentum}}.$$

In the above definition it is to be noted particularly that the polar angles θ, φ and solid angle $d\Omega$ refer to angles in $\underset{\sim}{x}$ space, not momentum space. The useful eigenfunction is that given by

$$(15.13)\quad \chi(\underset{\sim}{x}|\underset{\sim}{k}) = \chi_o(\underset{\sim}{x}|\underset{\sim}{k}) - \frac{em}{2\pi}\int \frac{e^{i|\underset{\sim}{k}|\,|\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x}-\underset{\sim}{x}'|}\, V(\underset{\sim}{x}')\chi(\underset{\sim}{x}|\underset{\sim}{k})d\underset{\sim}{x}'\ .$$

The incident wave corresponds to an incident particle with momentum k. The flux of incident particle through a surface normal to k is clearly,

$$(17.02)\quad \frac{|\underset{\sim}{k}|}{m}\,|\chi_o(\underset{\sim}{x}|\underset{\sim}{k})|^2 = \frac{|\underset{\sim}{k}|}{(2\pi)^3 m}$$

We shall calculate the numerator of (17.01) in the conventional fashion. We use the fact derived from the usual conservation of probability arguments that the rate of increase of the probability of finding a particle in a volume V, namely, $\frac{d}{dt}\int_V P(\underset{\sim}{x})\, d\underset{\sim}{x}$, where $P(\underset{\sim}{x})$ is the probability density, is related to the probability current by

$$\frac{d}{dt}\int_V P(\underset{\sim}{x})d\underset{\sim}{x} = -\int_S j_n dA \ . \tag{17.03}$$

In equation (17.03) the integration on the right is a surface integral taken over the surface bounding the volume V, and j_n is the component of the current $\underset{\sim}{j}$ normal to the surface element dA.

Now, if the volume V extends over all space the surface S may be taken to be the surface of a sphere which in the limit has an infinite radius. Writing $dA = |\underset{\sim}{x}|^2\, d\Omega$, we have, if V extends over all space,

$$\frac{d}{dt}\int P(\underset{\sim}{x})\, d\underset{\sim}{x} = -\int j_{|\underset{\sim}{x}|}\,(\theta,\varphi)\ |\underset{\sim}{x}|^2 d\Omega \tag{17.04}$$

where $j_{|\underset{\sim}{x}|}\,(\theta,\varphi)$ is the radial component of the current when $|\underset{\sim}{x}|$ is large and where θ, φ are the polar angles which give the direction of $\underset{\sim}{x}$. It is clear that we can interpret $j_{|\underset{\sim}{x}|}(\theta,\varphi)\ |\underset{\sim}{x}|^2 d\Omega$ as being the rate of increase of particles into the solid angle $d\Omega$. The current density is given in terms of the probability amplitudes $\Psi(\underset{\sim}{x})$ as follows

$$\underset{\sim}{j} = \frac{1}{2im}\left[\bar{\Psi}\ \underset{\sim}{\text{grad}}\ \Psi - \Psi\ \underset{\sim}{\text{grad}}\ \bar{\Psi}\right] \ . \tag{17.05}$$

In our case we are interested in using the scattered part of $\chi(\underset{\sim}{x}|\underset{\sim}{k})$ as the probability amplitude in order to calculate the numerator of (17.01). Since only the asymptotic form of the scattered part is needed, we use this form as given by (15.32), namely,

$$-(2\pi)^{1/2}\ em\ \frac{e^{i|\underset{\sim}{k}'|\ |\underset{\sim}{x}|}}{|\underset{\sim}{x}|}\ T^{p}_{\underset{\sim}{-}}(\underset{\sim}{k}'|\underset{\sim}{k}) \qquad \left(\underset{\sim}{k}' = |\underset{\sim}{k}|\ \frac{\underset{\sim}{x}}{|\underset{\sim}{x}|}\right) .$$

Substituting this expression into equation (17.05), we find that the numerator of (17.01) is

$$(17.06) \qquad j_{|\underset{\sim}{x}|}(\theta,\phi)\ |\underset{\sim}{x}|^2\ d\Omega = 2\pi\varepsilon^2 m\ |\underset{\sim}{k}|\ \ |T^{p}_{-}(\underset{\sim}{k}'|\underset{\sim}{k})|^2\ d\Omega\ .$$

Substituting (17.06) into the numerator of (17.01) and (17.02) into the denominator we obtain finally the well-known expression

$$(17.07) \qquad \sigma(\theta,\phi) = (2\pi)^4\ \varepsilon^2 m^2\ |T^{p}_{-}(\underset{\sim}{k}'|\underset{\sim}{k})\ |^2\ .$$

As mentioned above θ, ϕ refer to the direction in $\underset{\sim}{x}$ space. The direction of the vector $\underset{\sim}{k}'$ is also determined by these angles.

B. Definition in Terms of the Scattering Operator.

Before giving the definition of the cross-section in terms of the scattering operator we shall indicate how one can construct the probability that a particle lies in within solid angle $d\Omega$ in momentum space from the momentum representer of the state describing the particle. If we take $f(\underset{\sim}{p})$ as the momentum representer, then the probability of finding the particle in any region of momentum space is $\int |f(\underset{\sim}{p})|^2\ d\underset{\sim}{p}$. In particular, if one wished the probability within a solid angle $d\Omega$ in momentum space one introduces polar coordinates in momentum space and the differential $d\underset{\sim}{p} = |\underset{\sim}{p}|^2\ d|\underset{\sim}{p}|d\Omega$. Then it is clear the desired probability is

$$(17.08) \qquad \left[\int_0^{\infty} |\ f(\underset{\sim}{p})|^2\ |\underset{\sim}{p}|^2\ d|\underset{\sim}{p}|\ \right] d\Omega\ .$$

The definition of differential cross-section which we will use is motivated by the work of Friedrichs in reference 16, though we shall carry out the procedure in a more formal manner. The cross-section $\sigma(\theta,\phi)$ is defined by

$$(17.09) \qquad \sigma(\theta,\phi)d\Omega = \sigma_{in} \cdot (\text{probability of finding a particle in solid angle } d\Omega \text{ in momentum space}).$$

In (17.09) σ_{in} is the "incoming cross section." It is the reciprocal of the probability of finding an incident particle in a right cylinder of unit cross-section whose axis is in the direction of the momentum of the incoming particle. We should note that, in contrast to the previous definition, the polar angles θ, ϕ and solid angle $d\Omega$ now refer to the directions of the momentum.

We shall take as the incoming state $\overline{\Phi}_{-}$ an eigenstate of momentum corresponding to the value $\underset{\sim}{k}$. This is the same incoming state used in the

previous definition. Then

$$(17.10)\qquad \overline{\Phi}_- \underset{\underset{\sim}{p}}{\longleftrightarrow} f_-(\underset{\sim}{p}) = \delta(\underset{\sim}{p} - \underset{\sim}{k}) = \delta(p_x - k_x)\delta(p_y - k_y)\delta(p_z - k_z) \ .$$

We shall now calculate σ_{in} . For the purpose of this calculation let $\underset{\sim}{k}$ coincide with the z axis. Hence $k_x = k_y = 0$, $k_z = |\underset{\sim}{k}|$. The probability amplitude of finding an incident particle with z-component of momentum between p_z and $p_z + dp_z$ in the element of area dx dy is denoted by $\Psi_-(x,y,p_z)$. This amplitude is given by

$$\Psi_-(x,y,p_z) = \frac{1}{2\pi} \iint \delta(p_x)\delta(p_y)\, e^{ip_x x}\ e^{ip_y y}\, dp_x dp_y$$

$$\cdot\, \delta(p_z - |\underset{\sim}{k}|) = \frac{1}{2\pi}\ \delta(p_z - |\underset{\sim}{k}|) \ .$$

Hence the probability of finding an incident particle in the element of area dxdy is

$$(17.11)\qquad \left[\int_{-\infty}^{+\infty} |\Psi_-(x,y,p_z)\ |^2\, dp_z \right] dxdy$$

$$= \frac{1}{4\pi^2} \left[\int_{-\infty}^{+\infty} \delta(p_z - |\underset{\sim}{k}|)^2 dp_z \right] dx\, dy$$

$$= \left[\frac{1}{4\pi^2} \int_0^{\infty} \delta(|\underset{\sim}{p}| - |\underset{\sim}{k}|)^2\, d|\underset{\sim}{p}| \right] dx\, dy \ .$$

The second equation follows from the first by virtue of the fact that the δ-function vanishes identically when p_z is negative. Also, we have changed the notation for the variable of integration from p_z to $|\underset{\sim}{p}|$. The " value" of σ_{in} is thus

$$(17.12)\qquad \sigma_{in} = (2\pi)^2 \left[\int_0^{\infty} \delta(|\underset{\sim}{p}| - |\underset{\sim}{k}|)^2\, d|\underset{\sim}{p}| \right]^{-1} \ .$$

We must now find the probability of finding a particle in momentum space in the solid angle $d\Omega$. Using the scattering operator formalism, the state $\overline{\Phi}_+ = S\, \overline{\Phi}_-$ has the momentum representer $f_+(\underset{\sim}{p})$ where

$$(17.13) \qquad f_+(\underset{\sim}{p}) = \int S^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{p}')\, f_-(\underset{\sim}{p}')\, d\underset{\sim}{p}'$$

$$= S^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{k})$$

$$= \delta(\underset{\sim}{p} - \underset{\sim}{k}) - 2\pi i\varepsilon m\, |\underset{\sim}{p}|^{-1}\, \delta(|\underset{\sim}{p}| - |\underset{\sim}{k}|)\, T_-^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{\kappa})$$

using (17.10) and the form for $S^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{p}') = S(\underset{\sim}{p}|\underset{\sim}{p}')$ given by (16.24).

Let us now calculate the desired probability for the case that the polar angles θ, ϕ of $\underset{\sim}{p}$ are different from those of $\underset{\sim}{k}$. We can ignore the first term on the right of (17.13) since it is zero and according to (17.08) the desired probability is

$$(17.14) \qquad \left[\int_0^\infty |S^{\underset{\sim}{p}}(\underset{\sim}{p}|\underset{\sim}{k})|^2\, |\underset{\sim}{p}|^2\, d|\underset{\sim}{p}|\right] d\Omega$$

$$= (2\pi)^2\, \varepsilon^2 m^2\, |T_-^{\underset{\sim}{p}}(\underset{\sim}{k}'|\underset{\sim}{k})|^2 \left[\int_0^\infty |\underset{\sim}{p}|^{-2} |\underset{\sim}{p}|^2\, \delta(|\underset{\sim}{p}| - |\underset{\sim}{k}|)^2\, d|\underset{\sim}{p}|\right] d\Omega$$

$$= (2\pi)^2\, \varepsilon^2 m^2\, |\, T_-^{\underset{\sim}{p}}(\underset{\sim}{k}'|\underset{\sim}{k})|^2 \left[\int_0^\infty \delta(|\underset{\sim}{p}| - |\underset{\sim}{k}|)^2\, d|\underset{\sim}{p}|\right] d\Omega$$

where

$$\underset{\sim}{k}' = |\underset{\sim}{k}|\, \frac{\underset{\sim}{p}}{|\underset{\sim}{p}|} \quad .$$

Hence from (17.09) and (17.12)

$$(17.15) \qquad \sigma(\theta,\phi) = (2\pi)^4 \varepsilon^2 m^2\, |T_-^{\underset{\sim}{p}}(\underset{\sim}{k}'|\underset{\sim}{k})|^2 \quad .$$

The polar angles θ, ϕ refer to the direction of $\underset{\sim}{p}$ or equivalently of $\underset{\sim}{k}'$.

It is noted that the same expression is obtained as by the time-independent formalism, even though the two definitions were different.

In the above it might be objected that we have introduced the undefined concepts of the integral of the square of the δ-function of (17.12) and (17.14). However, the derivation could be made rigorous by letting $f_-(\underset{\sim}{p})$ of equation (17.10) be an approximate δ-function and after obtaining the expression for $\sigma(\theta,\phi)$, pass to the limit.

C. Time-Proportional Definition.

In the time-proportional definition we use our results for time-probabilities (section 13). Equation (13.08) states that if the state $\bar{\Phi}_-$ is an eigenstate of the Hamiltonian H_o (which in the present case is the kinetic energy operator T) corresponding to the eigenvalue E' and direction of momentum given by the polar angles θ', ϕ', i.e., if

$$(17.16) \quad \bar{\Phi}_- \underset{E}{\longleftrightarrow} f_-(E,\theta,\phi) = \delta(E-E')\delta(\theta-\theta')\delta(\phi-\phi'),$$

then the number of transitions per unit time into the energy range between E to E + dE and angular range between θ and $\theta + d\theta$ and ϕ and $\phi + d\phi$ is given by

$$(17.17) \quad W(E,\theta,\phi;t)dE\, d\theta d\phi = 2\pi\varepsilon^2\, \delta(E-E')\, |T_-(E,\theta,\phi|E',\theta',\phi')|^2 dE d\theta d\phi \ .$$

Hence the total number of transitions per unit time in the angular range between θ and $\theta + d\theta$ and ϕ and $\phi + d\phi$ is

$$(17.18) \quad \left[\int_0^\infty W(E,\theta,\phi;t)dE\right] d\theta d\phi = 2\pi\varepsilon^2\, |T_-(E',\theta,\phi|E',\theta',\phi')|^2 d\theta d\phi \ .$$

Since the solid angle $d\Omega$ in momentum space is $d\Omega = \sin\theta\, d\theta d\phi$ we can write (17.18) as

$$(17.18a) \quad \left[\int_0^\infty W(E,\theta,\phi;\, t)\right] (\sin\theta)^{-1}\, d\Omega$$

$$= 2\pi\varepsilon^2 |T_-(E',\theta,\phi|E',\, \theta',\phi')|^2\, (\sin\theta)^{-1}\, d\Omega$$

and interpret $\left[\int_0^\infty W(E,\theta,\phi;t)\right] (\sin\theta)^{-1}$ as

the number of transitions per unit time per unit solid angle.

We define $\sigma(\theta,\phi)$ as

$$(17.19) \quad \sigma(\theta,\phi)d\Omega = \frac{\text{number of transitions per unit time into } d\Omega}{\text{flux of incident particles through surface normal to momentum}} \ .$$

Let us calculate the denominator of the right hand side of the definition (17.19). In the $\underset{\sim}{x}$ representation the incident state (17.16) is given by

$$(17.20) \quad \bar{\Phi}_- \underset{\underset{\sim}{x}}{\longleftrightarrow} \chi_o(\underset{\sim}{x}|E',\theta',\phi') = (2m^3E')^{1/4}(\sin\theta')^{1/2}(\frac{1}{2\pi})^{3/2}\, e^{i(\underset{\sim}{k}\,\underset{\sim}{x})}$$

(see 15.06, 15.07, 15.08), where we take $\underset{\sim}{k}$ to be the momentum corresponding to

the energy and angles E', θ', ϕ'. The flux of incident particles through a surface normal to $\underset{\sim}{k}$ is

$$(17.21) \quad \frac{|\underset{\sim}{k}|}{m} |\chi_0(\underset{\sim}{x}|E',\theta',\phi')|^2 = \frac{|\underset{\sim}{k}|}{m} \frac{(2m^3E')^{1/2}\sin\theta'}{(2\pi)^3} \quad .$$

The numerator of the ratio in (17.19) is according to (17.18a), just

$$2\pi\epsilon^2 |T_-(E',\theta,\phi|E',\theta',\phi')|^2 (\sin\theta)^{-1} \, d\Omega \quad .$$

Hence

$$(17.22) \quad \sigma(\theta,\phi) = \frac{(2\pi)^4\epsilon^2 m \, |T_-(E',\theta,\phi|E',\theta',\phi')|^2}{|\underset{\sim}{k}| \, (2m^3E')^{1/2} \sin\theta \sin\theta'} \quad .$$

According to equation (15.33) we may write

$$T_-(E',\theta,\phi|E,\theta',\phi') = (2m^3E')^{1/2}(\sin\theta)^{1/2}(\sin\theta')^{1/2} T_-^{\underset{\sim}{p}}(\underset{\sim}{k}'|\underset{\sim}{k})$$

where $\underset{\sim}{k}'$ is the momentum vector corresponding to E', θ,ϕ . Note further that that

$$(17.23) \quad |k'| = |k| = \sqrt{2mE'} \quad .$$

Hence (17.22) becomes

$$(17.24) \quad \sigma(\theta,\phi) = \frac{(2\pi)^4\epsilon^2 m(2m^3E')^{1/2}|T_-^{\underset{\sim}{p}}(\underset{\sim}{k}'|\underset{\sim}{k})|^2}{|\underset{\sim}{k}|}$$

$$= (2\pi)^4\epsilon^2 m^2 |T_-^{\underset{\sim}{p}}(\underset{\sim}{k}'|\underset{\sim}{k})|^2$$

which has the same form obtained using the two previous definitions.

APPENDIX III

The Kohn-Hulthen Variational Principle

Equation (12.24) will first be proved. If $T_{\pm}$ is substituted for $\tilde{\mathcal{T}}_{\pm}$ in the expression (12.22) it is seen that $v_{\pm} = u_{\pm}$ so that

$$(III.1) \qquad I(T_{\pm}) = \lim_{F' \to F} \int_{E_a}^{E_b} \int u_{+}(E,\alpha|F',\beta')(H^{E}-F)u_{-}(E,\alpha|F,\beta)\,d\alpha\,dE \ .$$

Now since $u_{-}(E,\alpha|F,\beta)$ is an eigenfunction of H corresponding to the eigenvalue F in the H_o representation we have

$$(III.2) \qquad H^{E}\, u_{-}(E,\alpha|F,\beta) = F\, u_{-}(E,\alpha|F,\beta)$$

or

$$(III.3) \qquad (H^{E}-F)\, u_{-}(E,\alpha|F,\beta) = 0.$$

Equation (12.24) follows immediately.

We shall now show that the variation of $A(\tilde{\mathcal{T}}_{\pm})$, due to independent variations of $\tilde{\mathcal{T}}_{\pm}$ about $T_{\pm}$, vanish.

We denote the variation of $A(\tilde{\mathcal{T}}_{\pm})$ about $T_{\pm}$ by $\delta A(\tilde{\mathcal{T}}_{\pm})$ and have

$$(III.4) \qquad \delta A(\tilde{\mathcal{T}}_{\pm}) = A(T_{\pm} + \delta T_{\pm}) - A(T_{\pm}).$$

Using (12.19), (12.20) and (12.22) which give A, I and $v_{\pm}$ in terms of $T_{\pm}$ we have to the first order in $\delta T_{\pm}$ (noting that $I(T_{\pm}) = 0$)

$$(III.5) \qquad \delta A(\tilde{\mathcal{T}}_{\pm}) = \lim_{F' > F} \varepsilon \left[\int_{E_a}^{E_b} \int \bar{u}_{+}(E,\alpha|F',\beta')(H^{E}-F)\gamma_{-}(F-E)\delta T_{-}(E,\alpha|F,\beta)\,d\alpha\,dE \right.$$

$$\left. + \int_{E_a}^{E_b} \int \bar{\gamma}_{+}(F'-E)\overline{\delta T_{+}}(E,\alpha|F',\beta')(H^{E}-F)u_{-}(E,\alpha|F,\beta)\,d\alpha\,dE \right]$$

$$+ \varepsilon\, \delta T_{-}(F,\beta'|F,\beta).$$

The second integral on the right hand side of (III.5) vanishes because of (III.3).

The first integral is treated as follows. Let us designate the first integral by $A'(T_{\pm})$ where

$$(III.6)\quad A'(T_{\pm}) = \lim_{F'\to F} \varepsilon \int_{E_a}^{E_b}\int \bar{u}_+(E,\alpha|F',\beta')(H^E-F)\gamma_-(F-E)\delta T_-(E,\alpha|F,\beta)d\alpha dE.$$

Since H is a Hermitian operator and since u_+ is an eigenfunction of H so that we have in analogy to (III.2)

$$(III.2a)\qquad H^E u_+(E,\alpha|F',\beta') = F' u_+(E,\alpha|F',\beta'),$$

our expression for $A'(T_{\pm})$

$$A'(T_{\pm}) = \varepsilon \lim_{F'\to F} \int_{E_a}^{E_b}\int \left[\overline{(H^E-F)u_+(E,\alpha|F',\beta')}\right]\gamma_-(F-E)\delta T_-(E,\alpha|F,\beta)d\alpha dE$$

$$(III.7)\qquad = \varepsilon \lim_{F'\to F} \int_{E_a}^{E_b}\int \bar{u}_+(E,\alpha|F',\beta')(F'-F)\gamma_-(F-E)\delta T_-(E,\alpha|F,\beta)d\alpha dE\ .$$

We note that

$$(III.8)\qquad (F'-F)\gamma_-(F-E) = \left[(F'-E) - (F-E)\right]\gamma_-(F-E)$$

$$= (F'-E)\gamma_-(F-E) - (F-E)\gamma_-(F-E)$$

$$= (F'-E)\gamma_-(F-E) - 1\ .$$

Equation (III.7) is then

$$(III.9)\quad A'(T_{\pm}) = \varepsilon \lim_{F'\to F} \int_{E_a}^{E_b}\int \bar{u}_+(E,\alpha|F',\beta')(F'-E)\gamma_-(F-E)\delta T_-(E,\alpha|F,\beta)d\alpha dE$$

$$- \varepsilon \lim_{F'\to F} \int_{E_a}^{E_b}\int \bar{u}_+(E,\alpha|F',\beta')\delta T_-(E,\alpha|F,\beta)d\alpha dE$$

$$= \varepsilon \lim_{F'\to F} \int_{E_a}^{E_b}\int \varepsilon\, \bar{T}_+(E,\alpha|F',\beta')\gamma_-(F-E)\delta T_-(E,\alpha|F,\beta)d\alpha dE$$

$$- \varepsilon \lim_{F'\to F} \int_{E_a}^{E_b}\int \bar{u}_+(E,\alpha|F',\beta')\delta T_-(E,\alpha|F,\beta)d\alpha dF.$$

In (III.9) we have used the fact that $(F'-E)\, u_+(E,\alpha|F',\beta') = \varepsilon T_+(E,\alpha|F',\beta')$. In the first of the integrals we note that we no longer have products of symbolic functions. The only symbolic functions which appears is γ_-. The

functions T_+ and δT_- are proper functions. In the second integral $\bar{u}_+$ is a symbolic function but δT_- is not. Hence we can now interchange the limit and the integration processes. It was <u>not</u> permissible to do this earlier. Then recognizing that $\gamma_-(x) = \bar{\gamma}_+(x)$ we have

$$A'(T_{\pm}) = \varepsilon \int_{E_a}^{E_b} \int \varepsilon \bar{\gamma}_+(F-E)\ \bar{T}_+(E,\alpha|F,\beta')\delta T_-(E,\alpha|F,\beta)\,d\alpha\,dE \tag{III.10}$$

$$- \varepsilon \int_{E_a}^{E_b} \int \bar{u}_+(E,\alpha|F,\beta')\delta T_-(E,\alpha|F,\beta)\,d\alpha\,dE$$

From (6.27) we note that

$$\varepsilon\bar{\gamma}_+\ (F-E)\ \bar{T}_+(E,\alpha|F,\beta') = \bar{u}_+(E,\alpha|F,\beta') - \delta(E-F)\delta(\alpha,\beta').$$

Substituting this expression in the first term of the right hand member of (III.10) we have finally

$$A'(T_{\pm}) = -\varepsilon\delta T_-(F,\beta'|F,\beta) \tag{III.11}$$

so that from (III.5) we have

$$\delta A(\mathcal{T}_{\pm}) = 0 \tag{III.12}$$

as desired.

APPENDIX IV

An Alternative Expression for $A(\mathcal{J}_{\pm})$.

Substituting (12.21) which gives $v_{\pm}(E,\alpha|F,\beta)$ in terms of $\mathcal{J}_{\pm}$ $\mathcal{J}_{\pm}(E,\alpha|F,\beta)$ into $I(\mathcal{J}_{\pm})$ we have

$$(IV.1)\quad I(\mathcal{J}_{\pm}) = \lim_{F'\to F}\Big[\int_{E_a}^{E_b}\!\!\int \delta(E-F')\,\delta(\alpha,\beta')\,(H^E-F)\delta(E-F)\,\delta(\alpha,\beta)\,d\alpha dE$$

$$+ \varepsilon\int_{E_a}^{E_b}\!\!\int \bar{\gamma}_+(F'-E)\bar{\mathcal{J}}_+(E,\alpha|F',\beta')(H^E-F)\delta(E-F)\delta(\alpha,\beta)\,d\alpha dE$$

$$+ \varepsilon\int_{E_a}^{E_b}\!\!\int \delta(E-F')\delta(\alpha,\beta')(H^E-F)\gamma_-(F-E)\mathcal{J}_-(E,\alpha|F,\beta)\,d\alpha dE$$

$$+ \varepsilon^2\int_{E_a}^{E_b}\!\!\int \bar{\gamma}_+(F',E)\,\bar{\mathcal{J}}_+(E,\alpha|F',\beta')(H^E-F)\gamma_-(F-E)\mathcal{J}_-(E,\alpha|F,\beta)\,d\alpha dE\Big| \ .$$

Now $$H^E = H_o^E + V^E = E + V^E$$

so that $$(H^F - F)\,\delta(E-F)\,\delta(\alpha,\beta) = (E-F)\,\delta(F-F)\,\delta(\alpha,\beta) + \varepsilon V^E(E,\alpha|F,\beta)$$

$$= \varepsilon V^E(E,\alpha|F,\beta)$$

since $(E-F)\delta(E-F) = 0$ and $V^E\,\delta(E-F)\delta(\alpha,\beta) = \int_{E_a}^{E_b}\!\!\int V^E(E,\alpha|E',\alpha')\delta(E'-F)\delta(\alpha',\beta)\,d\alpha' dE'$

$= V^E(E,\alpha|F,\beta)$. Hence the first integral of (IV.1) is

$$\varepsilon\int_{E_a}^{E_b}\!\!\int \delta(E-F')\delta(\alpha,\beta')\ V^E(E,\alpha|F,\beta)\,d\alpha dE = \varepsilon V^E(F',\beta'|F,\beta) \ .$$

The second integral becomes, noting that $\bar{\gamma}_+(x) = \gamma_-(x)$,

$$\varepsilon\int_{E_a}^{E_b}\!\!\int \bar{\gamma}_+(F'-E)\,\bar{\mathcal{J}}_+(E,\alpha|F',\beta')\ V^E(E,\alpha|F,\beta)\,d\alpha dE$$

$$= \varepsilon\int_{E_a}^{E_b}\!\!\int \bar{\mathcal{J}}_+(E,\alpha|F',\beta')\gamma_-(F'-E)V^E(E,\alpha|F,\beta)\,d\alpha dE \ .$$

To rewrite the third integral we note that

$$(IV.3)\quad (H^E-F)\gamma_-(F-E)\mathcal{T}_-(E,\alpha|F,\beta) = (E-F)\gamma_-(F-E)\mathcal{T}_-(E,\alpha|F,\beta)+ \varepsilon V^E\gamma_-(F-E)\mathcal{T}_-(E,\alpha|F,\beta)$$

$$= -\mathcal{T}_-(E,\alpha|F,\beta) + \varepsilon\int_{E_a}^{E_b}\int V^E(E,\alpha|F',\alpha')\gamma_-(F-E')\mathcal{T}_-(E',\alpha'|F,\beta)d\alpha' dE' \ .$$

Hence the third integral is

$$-\int_{E_a}^{E_b}\int \delta(E-F')\delta(\alpha,\beta')\mathcal{T}_-(E,\alpha|F,\beta)d\alpha dE$$

$$+ \varepsilon\int_{E_a}^{E_b}\int\int_{E_a}^{E_b}\int \delta(E-F')\delta(\alpha,\beta')V^E(E,\alpha|E',\alpha')\gamma_-(F-E')\mathcal{T}_-(E',\alpha'|F,\beta)d\alpha' dE' d^{\alpha} dE$$

$$= -\mathcal{T}_-(F',\beta'|F,\beta) + \varepsilon\int_{E_a}^{E_b}\int V^E(F',\beta'|E,\alpha)\gamma_-(F-E)\mathcal{T}_-(E,\alpha|F,\beta)d\alpha dE.$$

The fourth integral is

$$-\int_{E_a}^{E_b}\int \bar{\mathcal{T}}_+(E,\alpha|F',\beta')\gamma_-(F'-E)\mathcal{T}_-(E,\alpha|F,\beta)d\alpha dE$$

$$+ \varepsilon\int_{E_a}^{E_b}\int\int_{E_a}^{E_b}\int \bar{\mathcal{T}}_+(E,\alpha|F',\beta')\gamma_-(F'-E)V^E(E,\alpha|E',\alpha')\gamma_-(F-E')\mathcal{T}_-(E',\alpha'|F,\beta)$$

$$\cdot\ d\alpha' dE' d^{\alpha} dE \ .$$

We can now take the limit as F' approaches F since none of the integrands contain products of symbolic functions of the same argument. Then $A(\mathcal{T}_{\pm})$ is given by

$$(IV.4)\quad A(\mathcal{T}_{\pm}) = I(\mathcal{T}_{\pm}) + \varepsilon\,\mathcal{T}_-(F,\beta'|F,\beta)$$

$$= \varepsilon\ V^E(F,\beta'|F,\beta) + \varepsilon^2\left[\int_{E_a}^{E_b}\int \bar{\mathcal{T}}_+(E,\alpha|F,\beta')\gamma_-(F-E)V^E(E,\alpha|F,\beta)d\alpha dE\right.$$

$$+\int_{E_a}^{E_b}\int V^{E}(F,\beta'|E,\alpha)\gamma_{-}(F-E)\tilde{J}_{-}(E,\alpha|F,\beta)\,d\alpha\,dE$$

$$-\int_{E_a}^{E_b}\int \tilde{J}_{+}(E,\alpha|F,\beta')\gamma_{-}(F-E)\tilde{J}_{-}(E,\alpha|F,\beta)\,d\alpha\,dE\Big]$$

$$+\varepsilon^{3}\int_{E_a}^{E_b}\int\int_{E_a}^{E_b}\int \tilde{J}_{+}(E,\alpha|F,\beta')\gamma_{-}(F-E)V^{E}(E,\alpha|E',\alpha')\gamma_{-}(F-E')$$

$$\cdot\ \tilde{J}_{-}(E',\alpha'|F,\beta)\,d\alpha'\,dE'\,d\alpha\,dE.$$

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* There is an error in the order of listing of references in Part I. In the list of references above this error has been corrected.

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